Pentaerythritol Tetranitrate

Other names:

1,3-Propanediol, 2,2-bis((nitrooxy)methyl)-, 1,3-dinitrate
1,3-Propanediol, 2,2-bis[(nitrooxy)methyl]-, dinitrate
1,3-Propanediol, 2,2-bis[(nitrooxy)methyl]-, dinitrate (ester)
2,2-Bis[(nitrooxy)methyl]-1,3-propanediol dinitrate (ester)
2,2-bis(hydroxymethyl)-1,3-propanediol tetranitrate
Angicap
Angitet
Antora
Arcotrate
Baritrate
C 2
C 2 (explosive)
CHOT
Cardiacap
Deltrate-20
Dilcoran-80
Dipentrate
Duotrate
Erinit
Extex
Hasethrol
Kaytrate
Lentrat
Lowetrate
Martrate-45
Metranil
Mycardol
Myotrate 10
Neo-Corovas
Neopentanetetrayl nitrate
Niperyt
Niperyth
Nitrinal
Nitrine
Nitro-Riletten
Nitrolong
Nitropent
Nitropenta
Nitropenta 7W
Nitropentaerythrite

Nitropentaerythritol
Nitropenton
Nitrotalans
P.E.T.N.
PETN
PETN (pentaerythritol tetranitrate)
Pen-Tetra
Pencard
Pentaerithrityl Tetranitrate
Pentaerythrityl tetranitrate
Pentafilin
Pentafin
Pentanitrine
Pentanitrol
Pentestan-80
Pentetrate Unicelles
Penthrit
Penthrite
Pentitrate
Pentral 80
Pentrate
Pentrinat
Pentrite
Pentritol
Pentritol tempules
Pentryate
Pergitral
Peridex
Peridex-LA
Peritrate
Perityl
Prevangor
Quintrate
Rythritol
Subicard
TEN
Tanipent
Tena
Tentrate-20
Terpate
Tetranitropentaerythrite
Tetranitropentaerythritol
Tetrasule

Tranite D-Lay
Vaso-80 Unicelles
Vasodiatol
Vasolat
XTX 8003

Inchi: InChI=1S/C5H8N4O12/c10-6(11)18-1-5(2-19-7(12)13,3-20-8(14)15)4-21-9(16)17/h1-4H2

InchiKey: TZRXHJWUDPFEEY-UHFFFAOYSA-N

Formula: C5H8N4O12

SMILES: O=[N+]([O-])OCC(CO[N+](=O)[O-])(CO[N+](=O)[O-])CO[N+](=O)[O-]

Mol. weight [g/mol]: 316.14

CAS: 78-11-5

Physical Properties

Property code	Value	Unit	Source
chs	-2569.80 ± 2.50	kJ/mol	NIST Webbook
chs	-2572.40 ± 0.80	kJ/mol	NIST Webbook
gf	-283.74	kJ/mol	Joback Method
hf	-727.20	kJ/mol	Joback Method
hfs	-538.50 ± 0.80	kJ/mol	NIST Webbook
hfus	51.49	kJ/mol	Joback Method
hsub	152.00 ± 2.00	kJ/mol	NIST Webbook
hsub	150.40 ± 1.30	kJ/mol	NIST Webbook
hvap	101.43	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	-1.194		Crippen Method
mcvol	174.470	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1805.54		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1813.94		NIST Webbook
rinpol	1805.54		NIST Webbook
tb	1007.61	K	Joback Method
tc	1272.59	K	Joback Method

tf	414.10	K	Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An investigation with HMX
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.50	J/mol×K	1007.61	Joback Method
cpg	542.46	J/mol×K	1051.77	Joback Method
cpg	545.06	J/mol×K	1095.94	Joback Method
cpg	546.27	J/mol×K	1140.10	Joback Method
cpg	546.09	J/mol×K	1184.26	Joback Method
cpg	544.50	J/mol×K	1228.43	Joback Method
cpg	541.50	J/mol×K	1272.59	Joback Method
hsubt	156.90 ± 0.80	kJ/mol	369.00	NIST Webbook
hsubt	151.90 ± 2.10	kJ/mol	390.50	NIST Webbook
psub	2.17e-05	kPa	353.30	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	9.50e-09	kPa	310.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	3.02e-08	kPa	315.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	1.64e-07	kPa	325.40	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	3.59e-07	kPa	329.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate

psub	7.31e-07	kPa	333.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	4.08e-06	kPa	343.30	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	5.41e-06	kPa	344.80	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	1.28e-05	kPa	350.10	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	2.31e-09	kPa	302.20	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	3.01e-05	kPa	356.10	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	3.53e-05	kPa	356.90	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	6.42e-05	kPa	361.10	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	7.50e-05	kPa	361.90	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	8.52e-05	kPa	363.20	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate

psub	1.77e-04	kPa	368.10	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	2.04e-04	kPa	368.90	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	2.08e-04	kPa	369.20	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	2.30e-04	kPa	370.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	3.42e-04	kPa	373.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	4.46e-04	kPa	374.90	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	4.86e-04	kPa	376.20	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	5.76e-04	kPa	376.60	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	7.62e-04	kPa	379.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	9.44e-04	kPa	380.50	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate

psub	9.58e-04	kPa	380.80	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate
psub	1.15e-03	kPa	382.00	Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate

Sources

Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An Investigation with PMMA	https://www.doi.org/10.1021/acs.jced.6b00769
Sublimation Pressure and Vapor Molecular Weight of Pentaerythritol Tetranitrate:	https://www.doi.org/10.1021/je0302203
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume