

Propionic acid, 3-iodo-, ethyl ester

Inchi:	InChI=1S/C5H9IO2/c1-2-8-5(7)3-4-6/h2-4H2,1H3
InchiKey:	KZTNQOAFISZIEI-UHFFFAOYSA-N
Formula:	C5H9IO2
SMILES:	CCOC(=O)CCI
Mol. weight [g/mol]:	228.03

Physical Properties

Property code	Value	Unit	Source
gf	-184.58	kJ/mol	Joback Method
hf	-314.46	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	45.25	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.375		Crippen Method
mvol	114.570	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1116.00		NIST Webbook
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tb	483.23	K	Joback Method
tc	696.06	K	Joback Method
tf	276.33	K	Joback Method
vc	0.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.12	J/molxK	483.23	Joback Method
cpg	213.80	J/molxK	518.70	Joback Method
cpg	222.07	J/molxK	554.17	Joback Method
cpg	229.94	J/molxK	589.64	Joback Method
cpg	237.42	J/molxK	625.12	Joback Method
cpg	244.50	J/molxK	660.59	Joback Method
cpg	251.21	J/molxK	696.06	Joback Method
dvisc	0.0036892	Paxs	276.33	Joback Method

dvisc	0.0020161	Paxs	310.81	Joback Method
dvisc	0.0012431	Paxs	345.30	Joback Method
dvisc	0.0008369	Paxs	379.78	Joback Method
dvisc	0.0006017	Paxs	414.26	Joback Method
dvisc	0.0004552	Paxs	448.75	Joback Method
dvisc	0.0003583	Paxs	483.23	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U406236&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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