

Propionic acid, 3-iodo-, isobutyl ester

Inchi:	InChI=1S/C7H13IO2/c1-6(2)5-10-7(9)3-4-8/h6H,3-5H2,1-2H3
InchiKey:	UKMGYUDNQFXVMF-UHFFFAOYSA-N
Formula:	C7H13IO2
SMILES:	CC(C)COC(=O)CCI
Mol. weight [g/mol]:	256.08

Physical Properties

Property code	Value	Unit	Source
gf	-170.18	kJ/mol	Joback Method
hf	-361.02	kJ/mol	Joback Method
hfus	17.56	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.011		Crippen Method
mcvol	142.750	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1274.00		NIST Webbook
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tb	528.55	K	Joback Method
tc	739.58	K	Joback Method
tf	283.87	K	Joback Method
vc	0.533	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.34	J/molxK	528.55	Joback Method
cpg	299.75	J/molxK	563.72	Joback Method
cpg	310.60	J/molxK	598.89	Joback Method
cpg	320.88	J/molxK	634.07	Joback Method
cpg	330.61	J/molxK	669.24	Joback Method
cpg	339.81	J/molxK	704.41	Joback Method
cpg	348.49	J/molxK	739.58	Joback Method
dvisc	0.0046711	Paxs	283.87	Joback Method

dvisc	0.0021715	Paxs	324.65	Joback Method
dvisc	0.0011976	Paxs	365.43	Joback Method
dvisc	0.0007444	Paxs	406.21	Joback Method
dvisc	0.0005046	Paxs	446.99	Joback Method
dvisc	0.0003650	Paxs	487.77	Joback Method
dvisc	0.0002776	Paxs	528.55	Joback Method

Sources

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=U406238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	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
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
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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