

Isobutyl 2,3-dichloropropanoate

Other names:	Propanoic acid, 2,3-dichloro, 2-methylpropyl ester
Inchi:	InChI=1S/C7H12Cl2O2/c1-5(2)4-11-7(10)6(9)3-8/h5-6H,3-4H2,1-2H3
InchiKey:	WHVMKUBKNGLRBV-UHFFFAOYSA-N
Formula:	C7H12Cl2O2
SMILES:	CC(C)COC(=O)C(Cl)CCl
Mol. weight [g/mol]:	199.07

Physical Properties

Property code	Value	Unit	Source
gf	-254.60	kJ/mol	Joback Method
hf	-474.65	kJ/mol	Joback Method
hfus	18.02	kJ/mol	Joback Method
hvap	48.33	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	2.032		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
ripol	1615.00		NIST Webbook
tb	509.83	K	Joback Method
tc	706.13	K	Joback Method
tf	270.65	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.25	J/molxK	509.83	Joback Method
cpg	302.21	J/molxK	542.55	Joback Method
cpg	312.68	J/molxK	575.26	Joback Method
cpg	322.65	J/molxK	607.98	Joback Method
cpg	332.13	J/molxK	640.70	Joback Method
cpg	341.13	J/molxK	673.41	Joback Method

cpg	349.65	J/molxK	706.13	Joback Method
dvisc	0.0052697	Paxs	270.65	Joback Method
dvisc	0.0022910	Paxs	310.51	Joback Method
dvisc	0.0012039	Paxs	350.38	Joback Method
dvisc	0.0007215	Paxs	390.24	Joback Method
dvisc	0.0004754	Paxs	430.10	Joback Method
dvisc	0.0003363	Paxs	469.97	Joback Method
dvisc	0.0002511	Paxs	509.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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