

Isobutyl 2-chloropropanoate

Inchi:	InChI=1S/C7H13ClO2/c1-5(2)4-10-7(9)6(3)8/h5-6H,4H2,1-3H3
InchiKey:	AEEGJNJYJCGJFZ-UHFFFAOYSA-N
Formula:	C7H13ClO2
SMILES:	CC(C)COC(=O)C(C)Cl
Mol. weight [g/mol]:	164.63

Physical Properties

Property code	Value	Unit	Source
gf	-242.67	kJ/mol	Joback Method
hf	-458.91	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	43.94	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.813		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	472.40	K	Joback Method
tc	663.16	K	Joback Method
tf	240.73	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.59	J/molxK	472.40	Joback Method
cpg	318.17	J/molxK	631.37	Joback Method
cpg	308.57	J/molxK	599.57	Joback Method
cpg	298.52	J/molxK	567.78	Joback Method
cpg	288.00	J/molxK	535.99	Joback Method
cpg	277.03	J/molxK	504.19	Joback Method
cpg	327.32	J/molxK	663.16	Joback Method
dvisc	0.0002547	Paxs	472.40	Joback Method
dvisc	0.0003433	Paxs	433.79	Joback Method
dvisc	0.0004906	Paxs	395.18	Joback Method

dvisc	0.0007574	Paxs	356.56	Joback Method
dvisc	0.0012993	Paxs	317.95	Joback Method
dvisc	0.0025878	Paxs	279.34	Joback Method
dvisc	0.0064287	Paxs	240.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004007&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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