Propionamide, 2,3-dichloro-N-isobutyl-

Inchi: InChI=1S/C7H13Cl2NO/c1-5(2)4-10-7(11)6(9)3-8/h5-6H,3-4H2,1-2H3,(H,10,11)
InchiKey: XXMYXWLLRMCYII-UHFFFAOYSA-N
Formula: C7H13Cl2NO
SMILES: CC(C)CNC(=O)C(Cl)CCl
Mol. weight [g/mol]: 198.09

Physical Properties

Property code	Value	Unit	Source
gf	-60.21	kJ/mol	Joback Method
hf	-288.96	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	52.35	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.605		Crippen Method
mcvol	145.520	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	537.58	K	Joback Method
tc	736.75	K	Joback Method
tf	301.08	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.83	J/mol×K	537.58	Joback Method
cpg	324.27	J/mol×K	570.78	Joback Method
cpg	335.10	J/mol×K	603.97	Joback Method
cpg	345.34	J/mol×K	637.17	Joback Method
cpg	355.00	J/mol×K	670.36	Joback Method
cpg	364.10	J/mol×K	703.56	Joback Method
cpg	372.67	J/mol×K	736.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U415223&Units=SI

Legend

cpg:	Ideal gas heat capacity
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