Propionamide, 2,3-dichloro-N-ethyl-

Inchi: InChI=1S/C5H9Cl2NO/c1-2-8-5(9)4(7)3-6/h4H,2-3H2,1H3,(H,8,9)
InchiKey: CMTAJZKYOJJXIN-UHFFFAOYSA-N
Formula: C5H9Cl2NO
SMILES: CCNC(=O)C(Cl)CCl
Mol. weight [g/mol]: 170.04

Physical Properties

Property code	Value	Unit	Source
gf	-74.61	kJ/mol	Joback Method
hf	-242.40	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	48.29	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	0.969		Crippen Method
mcvol	117.340	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	492.26	K	Joback Method
tc	692.62	K	Joback Method
tf	293.54	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.59	J/mol×K	492.26	Joback Method
cpg	236.64	J/mol×K	525.65	Joback Method
cpg	245.21	J/mol×K	559.05	Joback Method
cpg	253.31	J/mol×K	592.44	Joback Method
cpg	260.95	J/mol×K	625.83	Joback Method
cpg	268.16	J/mol×K	659.22	Joback Method
cpg	274.95	J/mol×K	692.62	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=U415221&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
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