Propionamide, 2,3-dichloro-N-butyl-

Inchi: InChI=1S/C7H13Cl2NO/c1-2-3-4-10-7(11)6(9)5-8/h6H,2-5H2,1H3,(H,10,11)
InchiKey: OLLVHCDDQQZUSG-UHFFFAOYSA-N
Formula: C7H13Cl2NO
SMILES: CCCCNC(=O)C(Cl)CCl
Mol. weight [g/mol]: 198.09

Physical Properties

Property code	Value	Unit	Source
gf	-57.77	kJ/mol	Joback Method
hf	-283.68	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.749		Crippen Method
mcvol	145.520	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1544.00		NIST Webbook
rinpol	1544.00		NIST Webbook
tb	538.02	K	Joback Method
tc	733.08	K	Joback Method
tf	316.08	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.49	J/mol×K	538.02	Joback Method
cpg	323.63	J/mol×K	570.53	Joback Method
cpg	334.19	J/mol×K	603.04	Joback Method
cpg	344.19	J/mol×K	635.55	Joback Method
cpg	353.65	J/mol×K	668.06	Joback Method
cpg	362.58	J/mol×K	700.57	Joback Method
cpg	371.01	J/mol×K	733.08	Joback Method

Sources

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=U415224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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