Propionamide, 2,3-dichloro-N-octyl-

Inchi: InChI=1S/C11H21Cl2NO/c1-2-3-4-5-6-7-8-14-11(15)10(13)9-12/h10H,2-9H2,1H3,(H,14,1
InchiKey: BCBUMXGYOTZXTN-UHFFFAOYSA-N
Formula: C11H21Cl2NO
SMILES: CCCCCCCCNC(=O)C(Cl)CCl
Mol. weight [g/mol]: 254.20

Physical Properties

Property code	Value	Unit	Source
gf	-24.09	kJ/mol	Joback Method
hf	-366.24	kJ/mol	Joback Method
hfus	35.81	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.309		Crippen Method
mcvol	201.880	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	629.54	K	Joback Method
tc	815.75	K	Joback Method
tf	361.16	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.61	J/mol×K	629.54	Joback Method
cpg	517.67	J/mol×K	660.57	Joback Method
cpg	531.01	J/mol×K	691.61	Joback Method
cpg	543.65	J/mol×K	722.64	Joback Method
cpg	555.63	J/mol×K	753.68	Joback Method
cpg	566.96	J/mol×K	784.71	Joback Method
cpg	577.66	J/mol×K	815.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415230&Units=SI
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

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