Propionamide, 2,3-dichloro-N-hexyl-

Inchi: InChI=1S/C9H17Cl2NO/c1-2-3-4-5-6-12-9(13)8(11)7-10/h8H,2-7H2,1H3,(H,12,13)
InchiKey: OAOXXCNINOHVHX-UHFFFAOYSA-N
Formula: C9H17Cl2NO
SMILES: CCCCCCNC(=O)C(Cl)CCl
Mol. weight [g/mol]: 226.14

Physical Properties

Property code	Value	Unit	Source
gf	-40.93	kJ/mol	Joback Method
hf	-324.96	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.529		Crippen Method
mcvol	173.700	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	583.78	K	Joback Method
tc	773.98	K	Joback Method
tf	338.62	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.76	J/mol×K	583.78	Joback Method
cpg	417.54	J/mol×K	615.48	Joback Method
cpg	429.67	J/mol×K	647.18	Joback Method
cpg	441.15	J/mol×K	678.88	Joback Method
cpg	452.03	J/mol×K	710.58	Joback Method
cpg	462.31	J/mol×K	742.28	Joback Method
cpg	472.01	J/mol×K	773.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415228&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

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