Propanamide, N,N-dihexyl-3-chloro-

Inchi: InChI=1S/C15H30ClNO/c1-3-5-7-9-13-17(15(18)11-12-16)14-10-8-6-4-2/h3-14H2,1-2H3
InchiKey: SIHRUMLFKNAMRI-UHFFFAOYSA-N
Formula: C15H30ClNO
SMILES: CCCCCCN(CCCCCC)C(=O)CCCl
Mol. weight [g/mol]: 275.86

Physical Properties

Property code	Value	Unit	Source
gf	45.35	kJ/mol	Joback Method
hf	-413.72	kJ/mol	Joback Method
hfus	43.42	kJ/mol	Joback Method
hvap	62.16	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.605		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	1969.00		NIST Webbook
tb	646.34	K	Joback Method
tc	817.60	K	Joback Method
tf	371.13	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.27	J/mol×K	646.34	Joback Method
cpg	682.45	J/mol×K	674.88	Joback Method
cpg	698.83	J/mol×K	703.43	Joback Method
cpg	714.43	J/mol×K	731.97	Joback Method
cpg	729.29	J/mol×K	760.52	Joback Method
cpg	743.43	J/mol×K	789.06	Joback Method
cpg	756.89	J/mol×K	817.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308502&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