Propanamide, N,N-dihexyl-2-chloro-

Inchi: InChI=1S/C15H30ClNO/c1-4-6-8-10-12-17(15(18)14(3)16)13-11-9-7-5-2/h14H,4-13H2,1-
InchiKey: CPIHTZXGVWMATK-UHFFFAOYSA-N
Formula: C15H30ClNO
SMILES: CCCCCCN(CCCCCC)C(=O)C(C)Cl
Mol. weight [g/mol]: 275.86

Physical Properties

Property code	Value	Unit	Source
gf	42.91	kJ/mol	Joback Method
hf	-419.00	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	61.77	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.603		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	1869.00		NIST Webbook
rinpol	1869.00		NIST Webbook
tb	645.90	K	Joback Method
tc	819.56	K	Joback Method
tf	356.13	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.67	J/mol×K	645.90	Joback Method
cpg	683.13	J/mol×K	674.84	Joback Method
cpg	699.75	J/mol×K	703.79	Joback Method
cpg	715.58	J/mol×K	732.73	Joback Method
cpg	730.63	J/mol×K	761.67	Joback Method
cpg	744.93	J/mol×K	790.61	Joback Method
cpg	758.53	J/mol×K	819.56	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=U308385&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