Propanamide, N,N-diheptyl-2-chloro-

Inchi: InChI=1S/C17H34ClNO/c1-4-6-8-10-12-14-19(17(20)16(3)18)15-13-11-9-7-5-2/h16H,4-1
InchiKey: UYMKAUWTCKPFKN-UHFFFAOYSA-N
Formula: C17H34ClNO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C(C)Cl
Mol. weight [g/mol]: 303.91

Physical Properties

Property code	Value	Unit	Source
gf	59.75	kJ/mol	Joback Method
hf	-460.28	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.383		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
pc	1259.27	kPa	Joback Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook
tb	691.66	K	Joback Method
tc	865.13	K	Joback Method
tf	378.67	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.31	J/mol×K	691.66	Joback Method
cpg	796.53	J/mol×K	720.57	Joback Method
cpg	813.87	J/mol×K	749.48	Joback Method
cpg	830.36	J/mol×K	778.39	Joback Method
cpg	846.04	J/mol×K	807.31	Joback Method
cpg	860.94	J/mol×K	836.22	Joback Method
cpg	875.10	J/mol×K	865.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308388&Units=SI

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