Propanamide, N-heptyl-N-octyl-2-chloro-

Inchi: InChI=1S/C18H36ClNO/c1-4-6-8-10-12-14-16-20(18(21)17(3)19)15-13-11-9-7-5-2/h17H,
InchiKey: QBZXHNDGBKWEQP-UHFFFAOYSA-N
Formula: C18H36ClNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)C(C)Cl
Mol. weight [g/mol]: 317.94

Physical Properties

Property code	Value	Unit	Source
gf	68.17	kJ/mol	Joback Method
hf	-480.92	kJ/mol	Joback Method
hfus	47.67	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.773		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2164.00		NIST Webbook
rinpol	2164.00		NIST Webbook
tb	714.54	K	Joback Method
tc	888.62	K	Joback Method
tf	389.94	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.34	J/mol×K	714.54	Joback Method
cpg	854.93	J/mol×K	743.55	Joback Method
cpg	872.61	J/mol×K	772.57	Joback Method
cpg	889.42	J/mol×K	801.58	Joback Method
cpg	905.39	J/mol×K	830.59	Joback Method
cpg	920.56	J/mol×K	859.60	Joback Method
cpg	934.97	J/mol×K	888.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308389&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