Propanamide, N-heptyl-N-octyl-3-chloro-

Inchi: InChI=1S/C18H36ClNO/c1-3-5-7-9-11-13-17-20(18(21)14-15-19)16-12-10-8-6-4-2/h3-17
InchiKey: BGTYIRFGMJZZQI-UHFFFAOYSA-N
Formula: C18H36ClNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)CCCl
Mol. weight [g/mol]: 317.94

Physical Properties

Property code	Value	Unit	Source
gf	70.61	kJ/mol	Joback Method
hf	-475.64	kJ/mol	Joback Method
hfus	51.19	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.775		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2265.00		NIST Webbook
tb	714.98	K	Joback Method
tc	887.41	K	Joback Method
tf	404.94	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.90	J/mol×K	714.98	Joback Method
cpg	854.28	J/mol×K	743.72	Joback Method
cpg	871.79	J/mol×K	772.46	Joback Method
cpg	888.45	J/mol×K	801.19	Joback Method
cpg	904.29	J/mol×K	829.93	Joback Method
cpg	919.36	J/mol×K	858.67	Joback Method
cpg	933.68	J/mol×K	887.41	Joback Method

Sources

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=U308506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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