Propanamide, N,N-diheptyl-3-chloro-

Inchi: InChI=1S/C17H34ClNO/c1-3-5-7-9-11-15-19(17(20)13-14-18)16-12-10-8-6-4-2/h3-16H2,
InchiKey: HMZMBEDMMYANJV-UHFFFAOYSA-N
Formula: C17H34ClNO
SMILES: CCCCCCCN(CCCCCCC)C(=O)CCCl
Mol. weight [g/mol]: 303.91

Physical Properties

Property code	Value	Unit	Source
gf	62.19	kJ/mol	Joback Method
hf	-455.00	kJ/mol	Joback Method
hfus	48.60	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.385		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
pc	1252.15	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	692.10	K	Joback Method
tc	863.66	K	Joback Method
tf	393.67	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.88	J/mol×K	692.10	Joback Method
cpg	795.87	J/mol×K	720.69	Joback Method
cpg	813.01	J/mol×K	749.29	Joback Method
cpg	829.33	J/mol×K	777.88	Joback Method
cpg	844.85	J/mol×K	806.47	Joback Method
cpg	859.63	J/mol×K	835.07	Joback Method
cpg	873.68	J/mol×K	863.66	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=U308505&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