Hexanamide, 6-chloro-N-ethyl-N-octyl-

Inchi: InChI=1S/C16H32ClNO/c1-3-5-6-7-8-12-15-18(4-2)16(19)13-10-9-11-14-17/h3-15H2,1-2
InchiKey: AEXPKITTWVZGCK-UHFFFAOYSA-N
Formula: C16H32ClNO
SMILES: CCCCCCCCN(CC)C(=O)CCCCCCl
Mol. weight [g/mol]: 289.88

Physical Properties

Property code	Value	Unit	Source
gf	53.77	kJ/mol	Joback Method
hf	-434.36	kJ/mol	Joback Method
hfus	46.01	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.995		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	669.22	K	Joback Method
tc	840.41	K	Joback Method
tf	382.40	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.98	J/mol×K	669.22	Joback Method
cpg	738.57	J/mol×K	697.75	Joback Method
cpg	755.33	J/mol×K	726.28	Joback Method
cpg	771.30	J/mol×K	754.82	Joback Method
cpg	786.51	J/mol×K	783.35	Joback Method
cpg	800.97	J/mol×K	811.88	Joback Method
cpg	814.74	J/mol×K	840.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415595&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