Hexanamide, 6-chloro-N-ethyl-N-2-ethylhexyl-

Inchi: InChI=1S/C16H32ClNO/c1-4-7-11-15(5-2)14-18(6-3)16(19)12-9-8-10-13-17/h15H,4-14H2
InchiKey: SFMJHCLAXLVSGA-UHFFFAOYSA-N
Formula: C16H32ClNO
SMILES: CCCCC(CC)CN(CC)C(=O)CCCCCCl
Mol. weight [g/mol]: 289.88

Physical Properties

Property code	Value	Unit	Source
gf	51.33	kJ/mol	Joback Method
hf	-439.64	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.851		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	668.78	K	Joback Method
tc	842.13	K	Joback Method
tf	367.40	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.40	J/mol×K	668.78	Joback Method
cpg	739.24	J/mol×K	697.67	Joback Method
cpg	756.23	J/mol×K	726.56	Joback Method
cpg	772.40	J/mol×K	755.45	Joback Method
cpg	787.78	J/mol×K	784.34	Joback Method
cpg	802.39	J/mol×K	813.24	Joback Method
cpg	816.28	J/mol×K	842.13	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=U415593&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