Propanamide, N,N-bis(2-ethylhexyl)-3-chloro-

Inchi: InChI=1S/C19H38ClNO/c1-5-9-11-17(7-3)15-21(19(22)13-14-20)16-18(8-4)12-10-6-2/h1
InchiKey: LJNYXXQVVFXPTJ-UHFFFAOYSA-N
Formula: C19H38ClNO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)CCCl
Mol. weight [g/mol]: 331.96

Physical Properties

Property code	Value	Unit	Source
gf	74.15	kJ/mol	Joback Method
hf	-506.84	kJ/mol	Joback Method
hfus	46.74	kJ/mol	Joback Method
hvap	70.29	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.877		Crippen Method
mcvol	302.360	ml/mol	McGowan Method
pc	1109.63	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	736.98	K	Joback Method
tc	913.70	K	Joback Method
tf	386.21	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.86	J/mol×K	736.98	Joback Method
cpg	915.00	J/mol×K	766.43	Joback Method
cpg	933.18	J/mol×K	795.89	Joback Method
cpg	950.44	J/mol×K	825.34	Joback Method
cpg	966.81	J/mol×K	854.80	Joback Method
cpg	982.34	J/mol×K	884.25	Joback Method
cpg	997.07	J/mol×K	913.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308504&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