Hexanamide, N,N-dioctyl-6-chloro-

Inchi: InChI=1S/C22H44ClNO/c1-3-5-7-9-11-16-20-24(21-17-12-10-8-6-4-2)22(25)18-14-13-15
InchiKey: YCAKAOFECFRADB-UHFFFAOYSA-N
Formula: C22H44ClNO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)CCCCCCl
Mol. weight [g/mol]: 374.04

Physical Properties

Property code	Value	Unit	Source
gf	104.29	kJ/mol	Joback Method
hf	-558.20	kJ/mol	Joback Method
hfus	61.55	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.335		Crippen Method
mcvol	344.630	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	806.50	K	Joback Method
tc	988.46	K	Joback Method
tf	450.02	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.70	J/mol×K	806.50	Joback Method
cpg	1097.85	J/mol×K	836.83	Joback Method
cpg	1116.96	J/mol×K	867.15	Joback Method
cpg	1135.08	J/mol×K	897.48	Joback Method
cpg	1152.26	J/mol×K	927.80	Joback Method
cpg	1168.54	J/mol×K	958.13	Joback Method
cpg	1183.98	J/mol×K	988.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308660&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