Hexanamide, N,N-dioctyl-

Other names: N,N-dioctyl hexanamide
Inchi: InChI=1S/C22H45NO/c1-4-7-10-12-14-17-20-23(22(24)19-16-9-6-3)21-18-15-13-11-8-5-
InchiKey: WRJVSLJKWITHBC-UHFFFAOYSA-N
Formula: C22H45NO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)CCCCC
Mol. weight [g/mol]: 339.60
CAS: 55334-54-8

Physical Properties

Property code	Value	Unit	Source
gf	116.22	kJ/mol	Joback Method
hf	-542.46	kJ/mol	Joback Method
hfus	88.08	kJ/mol	Enthalpies of vaporization of N,N-dialkyl monamides at 298.15K
hvap	88.10 ± 1.00	kJ/mol	NIST Webbook
log10ws	-7.38		Crippen Method
logp	7.116		Crippen Method
mcvol	332.390	ml/mol	McGowan Method
pc	935.77	kPa	Joback Method
tb	769.07	K	Joback Method
tc	943.91	K	Joback Method
tf	420.10	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.20	J/mol×K	769.07	Joback Method
cpg	1062.13	J/mol×K	798.21	Joback Method
cpg	1082.04	J/mol×K	827.35	Joback Method
cpg	1100.97	J/mol×K	856.49	Joback Method
cpg	1118.97	J/mol×K	885.63	Joback Method
cpg	1136.08	J/mol×K	914.77	Joback Method

cpg	1152.33	J/mol×K	943.91	Joback Method

Sources

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=C55334548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of vaporization of N,N-dialkyl monamides at 298.15K:	https://www.doi.org/10.1016/j.tca.2009.05.007

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume