

Hexanamide, 6-chloro-N-ethyl-N-dodecyl-

Inchi:	InChI=1S/C20H40ClNO/c1-3-5-6-7-8-9-10-11-12-16-19-22(4-2)20(23)17-14-13-15-18-21
InchiKey:	PYFDKGVXSSZXMQ-UHFFFAOYSA-N
Formula:	C20H40ClNO
SMILES:	CCCCCCCCCCCCN(CC)C(=O)CCCCCl
Mol. weight [g/mol]:	345.99

Physical Properties

Property code	Value	Unit	Source
gf	87.45	kJ/mol	Joback Method
hf	-516.92	kJ/mol	Joback Method
hfus	56.37	kJ/mol	Joback Method
hvap	73.29	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.555		Crippen Method
mvol	316.450	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
tb	760.74	K	Joback Method
tc	936.60	K	Joback Method
tf	427.48	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.99	J/mol×K	760.74	Joback Method
cpg	974.20	J/mol×K	790.05	Joback Method
cpg	992.47	J/mol×K	819.36	Joback Method
cpg	1009.82	J/mol×K	848.67	Joback Method
cpg	1026.30	J/mol×K	877.98	Joback Method
cpg	1041.96	J/mol×K	907.29	Joback Method
cpg	1056.82	J/mol×K	936.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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