

Hexanamide, N,N-didecyl-6-chloro-

Inchi:	InChI=1S/C26H52ClNO/c1-3-5-7-9-11-13-15-20-24-28(26(29)22-18-17-19-23-27)25-21-1
InchiKey:	PMKYWAKSSKVNKK-UHFFFAOYSA-N
Formula:	C26H52ClNO
SMILES:	CCCCCCCCCN(CCCCCCCCCC)C(=O)CCCCCl
Mol. weight [g/mol]:	430.15

Physical Properties

Property code	Value	Unit	Source
gf	137.97	kJ/mol	Joback Method
hf	-640.76	kJ/mol	Joback Method
hfus	71.91	kJ/mol	Joback Method
hvap	86.64	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	8.896		Crippen Method
mvol	400.990	ml/mol	McGowan Method
pc	734.42	kPa	Joback Method
rinpol	3029.00		NIST Webbook
tb	898.02	K	Joback Method
tc	1102.26	K	Joback Method
tf	495.10	K	Joback Method
vc	1.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.00	J/mol×K	898.02	Joback Method
cpg	1354.65	J/mol×K	932.06	Joback Method
cpg	1375.99	J/mol×K	966.10	Joback Method
cpg	1396.09	J/mol×K	1000.14	Joback Method
cpg	1415.04	J/mol×K	1034.18	Joback Method
cpg	1432.92	J/mol×K	1068.22	Joback Method
cpg	1449.80	J/mol×K	1102.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308662&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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