

Hexanamide, N,N-dibutyl-6-chloro-

Inchi:	InChI=1S/C14H28ClNO/c1-3-5-12-16(13-6-4-2)14(17)10-8-7-9-11-15/h3-13H2,1-2H3
InchiKey:	DLKRTZPVPJCJBW-UHFFFAOYSA-N
Formula:	C14H28ClNO
SMILES:	CCCCN(CCCC)C(=O)CCCCCl
Mol. weight [g/mol]:	261.83

Physical Properties

Property code	Value	Unit	Source
gf	36.93	kJ/mol	Joback Method
hf	-393.08	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	59.93	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.214		Crippen Method
mvol	231.910	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	1852.00		NIST Webbook
rinpol	1852.00		NIST Webbook
tb	623.46	K	Joback Method
tc	795.18	K	Joback Method
tf	359.86	K	Joback Method
vc	0.892	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.85	J/mol×K	623.46	Joback Method
cpg	627.59	J/mol×K	652.08	Joback Method
cpg	643.55	J/mol×K	680.70	Joback Method
cpg	658.76	J/mol×K	709.32	Joback Method
cpg	673.25	J/mol×K	737.94	Joback Method
cpg	687.04	J/mol×K	766.56	Joback Method
cpg	700.16	J/mol×K	795.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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