

Hexanamide, N-ethyl-N-2-ethylhexyl-

Inchi:	InChI=1S/C16H33NO/c1-5-9-11-13-16(18)17(8-4)14-15(7-3)12-10-6-2/h15H,5-14H2,1-4H
InchiKey:	MBQDOAMCSJSAFJ-UHFFFAOYSA-N
Formula:	C16H33NO
SMILES:	CCCCC(=O)N(CC)CC(CC)CCCC
Mol. weight [g/mol]:	255.44

Physical Properties

Property code	Value	Unit	Source
gf	63.26	kJ/mol	Joback Method
hf	-423.90	kJ/mol	Joback Method
hfus	38.29	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.632		Crippen Method
mvol	247.850	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	631.35	K	Joback Method
tc	799.87	K	Joback Method
tf	337.48	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.65	J/molxK	631.35	Joback Method
cpg	704.37	J/molxK	659.44	Joback Method
cpg	722.24	J/molxK	687.52	Joback Method
cpg	739.30	J/molxK	715.61	Joback Method
cpg	755.57	J/molxK	743.70	Joback Method
cpg	771.08	J/molxK	771.78	Joback Method
cpg	785.85	J/molxK	799.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U415423&Units=SI

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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