

Hexanamide, N-ethyl-N-octyl-

Inchi:	InChI=1S/C16H33NO/c1-4-7-9-10-11-13-15-17(6-3)16(18)14-12-8-5-2/h4-15H2,1-3H3
InchiKey:	HGYSGTASMVRYJX-UHFFFAOYSA-N
Formula:	C16H33NO
SMILES:	CCCCCCCCN(CC)C(=O)CCCC
Mol. weight [g/mol]:	255.44

Physical Properties

Property code	Value	Unit	Source
gf	65.70	kJ/mol	Joback Method
hf	-418.62	kJ/mol	Joback Method
hfus	41.82	kJ/mol	Joback Method
hvap	60.00	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.776		Crippen Method
mvol	247.850	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook
tb	631.79	K	Joback Method
tc	798.03	K	Joback Method
tf	352.48	K	Joback Method
vc	0.956	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.29	J/mol×K	631.79	Joback Method
cpg	703.72	J/mol×K	659.50	Joback Method
cpg	721.33	J/mol×K	687.20	Joback Method
cpg	738.15	J/mol×K	714.91	Joback Method
cpg	754.21	J/mol×K	742.62	Joback Method
cpg	769.54	J/mol×K	770.33	Joback Method
cpg	784.16	J/mol×K	798.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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