

Hexanamide, N-ethyl

Inchi:	InChI=1S/C8H17NO/c1-3-5-6-7-8(10)9-4-2/h3-7H2,1-2H3,(H,9,10)
InchiKey:	BZWNNMQUYVVGJM-UHFFFAOYSA-N
Formula:	C8H17NO
SMILES:	CCCCCC(=O)NCC
Mol. weight [g/mol]:	143.23

Physical Properties

Property code	Value	Unit	Source
gf	-23.05	kJ/mol	Joback Method
hf	-267.56	kJ/mol	Joback Method
hfus	23.17	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.703		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinqol	1216.00		NIST Webbook
tb	486.48	K	Joback Method
tc	665.17	K	Joback Method
tf	282.51	K	Joback Method
vc	0.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.21	J/mol×K	486.48	Joback Method
cpg	315.13	J/mol×K	516.26	Joback Method
cpg	327.51	J/mol×K	546.04	Joback Method
cpg	339.35	J/mol×K	575.82	Joback Method
cpg	350.67	J/mol×K	605.60	Joback Method
cpg	361.49	J/mol×K	635.38	Joback Method
cpg	371.81	J/mol×K	665.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R50690&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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