

Pentanamide, N,N-dihexyl-

Inchi:	InChI=1S/C17H35NO/c1-4-7-10-12-15-18(16-13-11-8-5-2)17(19)14-9-6-3/h4-16H2,1-3H1
InchiKey:	JMPFRSTVOKJKHS-UHFFFAOYSA-N
Formula:	C17H35NO
SMILES:	CCCCCN(CCCCC)C(=O)CCCC
Mol. weight [g/mol]:	269.47

Physical Properties

Property code	Value	Unit	Source
gf	74.12	kJ/mol	Joback Method
hf	-439.26	kJ/mol	Joback Method
hfus	44.41	kJ/mol	Joback Method
hvap	62.23	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	5.166		Crippen Method
mvol	261.940	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	654.67	K	Joback Method
tc	821.09	K	Joback Method
tf	363.75	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.88	J/molxK	654.67	Joback Method
cpg	760.70	J/molxK	682.41	Joback Method
cpg	778.69	J/molxK	710.14	Joback Method
cpg	795.87	J/molxK	737.88	Joback Method
cpg	812.26	J/molxK	765.62	Joback Method
cpg	827.90	J/molxK	793.35	Joback Method
cpg	842.81	J/molxK	821.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308180&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
hvap:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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