

Pentanamide, N,N-diheptyl-

Inchi:	InChI=1S/C19H39NO/c1-4-7-10-12-14-17-20(19(21)16-9-6-3)18-15-13-11-8-5-2/h4-18H2
InchiKey:	OZNLXIWBUIWGSS-UHFFFAOYSA-N
Formula:	C19H39NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)CCCC
Mol. weight [g/mol]:	297.52

Physical Properties

Property code	Value	Unit	Source
gf	90.96	kJ/mol	Joback Method
hf	-480.54	kJ/mol	Joback Method
hfus	49.59	kJ/mol	Joback Method
hvap	66.68	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.946		Crippen Method
mvol	290.120	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	2115.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	700.43	K	Joback Method
tc	868.54	K	Joback Method
tf	386.29	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.55	J/mol×K	700.43	Joback Method
cpg	878.17	J/mol×K	728.45	Joback Method
cpg	896.89	J/mol×K	756.47	Joback Method
cpg	914.75	J/mol×K	784.49	Joback Method
cpg	931.77	J/mol×K	812.50	Joback Method
cpg	947.99	J/mol×K	840.52	Joback Method
cpg	963.44	J/mol×K	868.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308183&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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