

Butanamide, N,N-diheptyl-

Inchi:	InChI=1S/C18H37NO/c1-4-7-9-11-13-16-19(18(20)15-6-3)17-14-12-10-8-5-2/h4-17H2,1-
InchiKey:	QUIAENUAGVJHSB-UHFFFAOYSA-N
Formula:	C18H37NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)CCC
Mol. weight [g/mol]:	283.49

Physical Properties

Property code	Value	Unit	Source
gf	82.54	kJ/mol	Joback Method
hf	-459.90	kJ/mol	Joback Method
hfus	47.00	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.556		Crippen Method
mcvol	276.030	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinqol	1979.00		NIST Webbook
tb	677.55	K	Joback Method
tc	844.58	K	Joback Method
tf	375.02	K	Joback Method
vc	1.067	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.65	J/molxK	677.55	Joback Method
cpg	818.88	J/molxK	705.39	Joback Method
cpg	837.23	J/molxK	733.23	Joback Method
cpg	854.75	J/molxK	761.06	Joback Method
cpg	871.46	J/molxK	788.90	Joback Method
cpg	887.39	J/molxK	816.74	Joback Method
cpg	902.58	J/molxK	844.58	Joback Method

Sources

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=U308679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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