Propanamide, N,N-diheptyl-2,2-dimethyl-

Inchi: InChI=1S/C19H39NO/c1-6-8-10-12-14-16-20(18(21)19(3,4)5)17-15-13-11-9-7-2/h6-17H2
InchiKey: WMFVDRIGDVTEIA-UHFFFAOYSA-N
Formula: C19H39NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C(C)(C)C
Mol. weight [g/mol]: 297.52

Physical Properties

Property code	Value	Unit	Source
gf	93.80	kJ/mol	Joback Method
hf	-489.29	kJ/mol	Joback Method
hfus	42.17	kJ/mol	Joback Method
hvap	65.38	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.802		Crippen Method
mcvol	290.120	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2009.00		NIST Webbook
tb	697.20	K	Joback Method
tc	869.84	K	Joback Method
tf	388.71	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.35	J/mol×K	697.20	Joback Method
cpg	880.32	J/mol×K	725.97	Joback Method
cpg	899.32	J/mol×K	754.75	Joback Method
cpg	917.39	J/mol×K	783.52	Joback Method
cpg	934.57	J/mol×K	812.29	Joback Method
cpg	950.91	J/mol×K	841.06	Joback Method
cpg	966.46	J/mol×K	869.84	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=U308128&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
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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