Propanamide, N,N-dihexyl-2,2-dimethyl-

Inchi: InChI=1S/C17H35NO/c1-6-8-10-12-14-18(15-13-11-9-7-2)16(19)17(3,4)5/h6-15H2,1-5H3
InchiKey: HDBMDSBFRNAGDL-UHFFFAOYSA-N
Formula: C17H35NO
SMILES: CCCCCCN(CCCCCC)C(=O)C(C)(C)C
Mol. weight [g/mol]: 269.47

Physical Properties

Property code	Value	Unit	Source
gf	76.96	kJ/mol	Joback Method
hf	-448.01	kJ/mol	Joback Method
hfus	36.99	kJ/mol	Joback Method
hvap	60.93	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	5.022		Crippen Method
mcvol	261.940	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	651.44	K	Joback Method
tc	823.82	K	Joback Method
tf	366.17	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.10	J/mol×K	651.44	Joback Method
cpg	763.48	J/mol×K	680.17	Joback Method
cpg	781.92	J/mol×K	708.90	Joback Method
cpg	799.45	J/mol×K	737.63	Joback Method
cpg	816.12	J/mol×K	766.36	Joback Method
cpg	831.97	J/mol×K	795.09	Joback Method
cpg	847.04	J/mol×K	823.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308126&Units=SI
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

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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