Propanamide, N,N-dihexyl-2-methyl-

Inchi: InChI=1S/C16H33NO/c1-5-7-9-11-13-17(16(18)15(3)4)14-12-10-8-6-2/h15H,5-14H2,1-4H
InchiKey: DNDXYYRWIVBWAP-UHFFFAOYSA-N
Formula: C16H33NO
SMILES: CCCCCCN(CCCCCC)C(=O)C(C)C
Mol. weight [g/mol]: 255.44

Physical Properties

Property code	Value	Unit	Source
gf	63.26	kJ/mol	Joback Method
hf	-423.90	kJ/mol	Joback Method
hfus	38.29	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.632		Crippen Method
mcvol	247.850	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	1768.00		NIST Webbook
tb	631.35	K	Joback Method
tc	799.87	K	Joback Method
tf	337.48	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.65	J/mol×K	631.35	Joback Method
cpg	704.37	J/mol×K	659.44	Joback Method
cpg	722.24	J/mol×K	687.52	Joback Method
cpg	739.30	J/mol×K	715.61	Joback Method
cpg	755.57	J/mol×K	743.70	Joback Method
cpg	771.08	J/mol×K	771.78	Joback Method
cpg	785.85	J/mol×K	799.87	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=U308082&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
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