Propanamide, N,N-diheptyl-2-methyl-

Inchi: InChI=1S/C18H37NO/c1-5-7-9-11-13-15-19(18(20)17(3)4)16-14-12-10-8-6-2/h17H,5-16H
InchiKey: RLNVEUZTQKJWMH-UHFFFAOYSA-N
Formula: C18H37NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C(C)C
Mol. weight [g/mol]: 283.49

Physical Properties

Property code	Value	Unit	Source
gf	80.10	kJ/mol	Joback Method
hf	-465.18	kJ/mol	Joback Method
hfus	43.47	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.412		Crippen Method
mcvol	276.030	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	1961.00		NIST Webbook
tb	677.11	K	Joback Method
tc	845.94	K	Joback Method
tf	360.02	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.05	J/mol×K	677.11	Joback Method
cpg	819.51	J/mol×K	705.25	Joback Method
cpg	838.08	J/mol×K	733.39	Joback Method
cpg	855.79	J/mol×K	761.53	Joback Method
cpg	872.66	J/mol×K	789.66	Joback Method
cpg	888.73	J/mol×K	817.80	Joback Method
cpg	904.04	J/mol×K	845.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308085&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