Propanamide, N-heptyl-N-octyl-2-methyl-

Inchi: InChI=1S/C19H39NO/c1-5-7-9-11-13-15-17-20(19(21)18(3)4)16-14-12-10-8-6-2/h18H,5-
InchiKey: WQWFHJBKCSBTFW-UHFFFAOYSA-N
Formula: C19H39NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)C(C)C
Mol. weight [g/mol]: 297.52

Physical Properties

Property code	Value	Unit	Source
gf	88.52	kJ/mol	Joback Method
hf	-485.82	kJ/mol	Joback Method
hfus	46.06	kJ/mol	Joback Method
hvap	66.29	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.802		Crippen Method
mcvol	290.120	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2061.00		NIST Webbook
tb	699.99	K	Joback Method
tc	869.66	K	Joback Method
tf	371.29	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.96	J/mol×K	699.99	Joback Method
cpg	878.79	J/mol×K	728.27	Joback Method
cpg	897.69	J/mol×K	756.55	Joback Method
cpg	915.71	J/mol×K	784.82	Joback Method
cpg	932.87	J/mol×K	813.10	Joback Method
cpg	949.21	J/mol×K	841.38	Joback Method
cpg	964.76	J/mol×K	869.66	Joback Method

Sources

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=U308086&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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