Propanamide, N-heptyl-N-octyl-2,2-dimethyl-

Inchi: InChI=1S/C20H41NO/c1-6-8-10-12-14-16-18-21(19(22)20(3,4)5)17-15-13-11-9-7-2/h6-18
InchiKey: CBOCKIPUKOQCTH-UHFFFAOYSA-N
Formula: C20H41NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)C(C)(C)C
Mol. weight [g/mol]: 311.55

Physical Properties

Property code	Value	Unit	Source
gf	102.22	kJ/mol	Joback Method
hf	-509.93	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	6.192		Crippen Method
mcvol	304.210	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	720.08	K	Joback Method
tc	893.57	K	Joback Method
tf	399.98	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.05	J/mol×K	720.08	Joback Method
cpg	940.33	J/mol×K	749.00	Joback Method
cpg	959.61	J/mol×K	777.91	Joback Method
cpg	977.95	J/mol×K	806.83	Joback Method
cpg	995.38	J/mol×K	835.74	Joback Method
cpg	1011.97	J/mol×K	864.66	Joback Method
cpg	1027.75	J/mol×K	893.57	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=U308129&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