Propanamide, 2-methyl-N-ethyl-N-octyl-

Inchi: InChI=1S/C14H29NO/c1-5-7-8-9-10-11-12-15(6-2)14(16)13(3)4/h13H,5-12H2,1-4H3
InchiKey: SASLAUPCKIWKEU-UHFFFAOYSA-N
Formula: C14H29NO
SMILES: CCCCCCCCN(CC)C(=O)C(C)C
Mol. weight [g/mol]: 227.39

Physical Properties

Property code	Value	Unit	Source
gf	46.42	kJ/mol	Joback Method
hf	-382.62	kJ/mol	Joback Method
hfus	33.11	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.851		Crippen Method
mcvol	219.670	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	585.59	K	Joback Method
tc	755.26	K	Joback Method
tf	314.94	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.37	J/mol×K	585.59	Joback Method
cpg	594.24	J/mol×K	613.87	Joback Method
cpg	611.32	J/mol×K	642.15	Joback Method
cpg	627.62	J/mol×K	670.42	Joback Method
cpg	643.18	J/mol×K	698.70	Joback Method
cpg	658.02	J/mol×K	726.98	Joback Method
cpg	672.17	J/mol×K	755.26	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=U415346&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