Valeramide, 3-hydroxy-2,2,4-trimethyl

Inchi: InChI=1S/C8H17NO2/c1-5(2)6(10)8(3,4)7(9)11/h5-6,10H,1-4H3,(H2,9,11)
InchiKey: NEDAPQCBLYSKRZ-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CC(C)C(O)C(C)(C)C(N)=O
Mol. weight [g/mol]: 159.23
CAS: 90227-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-184.85	kJ/mol	Joback Method
hf	-458.78	kJ/mol	Joback Method
hfus	12.90	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	0.515		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
tb	596.91	K	Joback Method
tc	791.44	K	Joback Method
tf	346.35	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.29	J/mol×K	596.91	Joback Method
cpg	383.18	J/mol×K	629.33	Joback Method
cpg	394.38	J/mol×K	661.75	Joback Method
cpg	404.92	J/mol×K	694.18	Joback Method
cpg	414.83	J/mol×K	726.60	Joback Method
cpg	424.16	J/mol×K	759.02	Joback Method
cpg	432.92	J/mol×K	791.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90227433&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume