N-ethyl-2,2,4-trimethyl-3-oxo-valeramide

Inchi: InChI=1S/C10H19NO2/c1-6-11-9(13)10(4,5)8(12)7(2)3/h7H,6H2,1-5H3,(H,11,13)
InchiKey: BNKHVNVYVPGXLW-UHFFFAOYSA-N
Formula: C10H19NO2
SMILES: CCNC(=O)C(C)(C)C(=O)C(C)C
Mol. weight [g/mol]: 185.26
CAS: 33471-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-134.73	kJ/mol	Joback Method
hf	-435.45	kJ/mol	Joback Method
hfus	19.02	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.374		Crippen Method
mcvol	164.880	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	582.44	K	Joback Method
tc	779.87	K	Joback Method
tf	342.40	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.49	J/mol×K	582.44	Joback Method
cpg	434.11	J/mol×K	615.34	Joback Method
cpg	447.89	J/mol×K	648.25	Joback Method
cpg	460.86	J/mol×K	681.15	Joback Method
cpg	473.06	J/mol×K	714.06	Joback Method
cpg	484.53	J/mol×K	746.96	Joback Method
cpg	495.30	J/mol×K	779.87	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=C33471691&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume