Valeramide, n-tert-butyl-2,2,4-trimethyl-3-oxo-

Inchi: InChI=1S/C12H23NO2/c1-8(2)9(14)12(6,7)10(15)13-11(3,4)5/h8H,1-7H3,(H,13,15)
InchiKey: NOAPYXCKEOPLNN-UHFFFAOYSA-N
Formula: C12H23NO2
SMILES: CC(C)C(=O)C(C)(C)C(=O)NC(C)(C)C
Mol. weight [g/mol]: 213.32
CAS: 16478-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-115.05	kJ/mol	Joback Method
hf	-485.48	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.152		Crippen Method
mcvol	193.060	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
tb	624.97	K	Joback Method
tc	827.72	K	Joback Method
tf	367.36	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.09	J/mol×K	624.97	Joback Method
cpg	539.48	J/mol×K	658.76	Joback Method
cpg	554.82	J/mol×K	692.55	Joback Method
cpg	569.18	J/mol×K	726.34	Joback Method
cpg	582.61	J/mol×K	760.13	Joback Method
cpg	595.19	J/mol×K	793.92	Joback Method
cpg	606.96	J/mol×K	827.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16478845&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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