

Valeramide, n-cyclohexyl-2,2,4-trimethyl-3-oxo-

Inchi:	InChI=1S/C14H25NO2/c1-10(2)12(16)14(3,4)13(17)15-11-8-6-5-7-9-11/h10-11H,5-9H2,1
InchiKey:	YUYDQLGDIIVEKR-UHFFFAOYSA-N
Formula:	C14H25NO2
SMILES:	CC(C)C(=O)C(C)(C)C(=O)NC1CCCCC1
Mol. weight [g/mol]:	239.35
CAS:	24388-84-9

Physical Properties

Property code	Value	Unit	Source
gf	-76.60	kJ/mol	Joback Method
hf	-463.69	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	65.43	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.687		Crippen Method
mcvol	210.380	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
tb	693.51	K	Joback Method
tc	910.79	K	Joback Method
tf	394.86	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.95	J/molxK	693.51	Joback Method
cpg	638.97	J/molxK	729.72	Joback Method
cpg	656.67	J/molxK	765.94	Joback Method
cpg	673.11	J/molxK	802.15	Joback Method
cpg	688.36	J/molxK	838.36	Joback Method
cpg	702.48	J/molxK	874.57	Joback Method
cpg	715.55	J/molxK	910.79	Joback Method

Sources

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=C24388849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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