

Alpha,alpha'-diacetyl-glutaramide

Inchi:	InChI=1S/C9H14N2O4/c1-4(12)6(8(10)14)3-7(5(2)13)9(11)15/h6-7H,3H2,1-2H3,(H2,10,1
InchiKey:	JYWFWVICVDCUDP-UHFFFAOYSA-N
Formula:	C9H14N2O4
SMILES:	CC(=O)C(CC(C(C)=O)C(N)=O)C(N)=O
Mol. weight [g/mol]:	214.22
CAS:	90566-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-362.76	kJ/mol	Joback Method
hf	-622.39	kJ/mol	Joback Method
hfus	28.81	kJ/mol	Joback Method
hvap	83.12	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	-1.242		Crippen Method
mcvol	163.910	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	764.98	K	Joback Method
tc	985.80	K	Joback Method
tf	527.43	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.60	J/molxK	764.98	Joback Method
cpg	471.63	J/molxK	801.78	Joback Method
cpg	480.87	J/molxK	838.59	Joback Method
cpg	489.36	J/molxK	875.39	Joback Method
cpg	497.10	J/molxK	912.19	Joback Method
cpg	504.13	J/molxK	948.99	Joback Method
cpg	510.47	J/molxK	985.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90566306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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