

[1,1'-Bicyclohexyl]-2-one, 1'-hydroxy-

Other names:	1'-hydroxy-[1,1'-bicyclohexyl]-2-one 2-(1'-Hydroxycyclohexyl)cyclohexanone
Inchi:	InChI=1S/C12H20O2/c13-11-7-3-2-6-10(11)12(14)8-4-1-5-9-12/h10,14H,1-9H2
InchiKey:	AERVJOBGBMEFDV-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	O=C1CCCCC1C1(O)CCCCC1
Mol. weight [g/mol]:	196.29
CAS:	28746-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-165.84	kJ/mol	Joback Method
hf	-457.06	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Thermodynamic Properties for 2-(1'-Hydroxycyclohexyl)cyclohexanone and Equilibrium of Dimerization of Cyclohexanone
hvap	62.94	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.441		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	673.30	K	Joback Method
tc	907.47	K	Joback Method
tf	392.70	K	Joback Method
vc	0.598	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.03	J/mol×K	829.42	Joback Method
cpg	583.97	J/mol×K	868.45	Joback Method
cpg	495.44	J/mol×K	673.30	Joback Method

cpg	515.16	J/mol×K	712.33	Joback Method
cpg	533.75	J/mol×K	751.36	Joback Method
cpg	551.34	J/mol×K	790.39	Joback Method
cpg	599.27	J/mol×K	907.47	Joback Method
hfust	20.81	kJ/mol	157.50	NIST Webbook
hvapt	87.74	kJ/mol	303.11	Thermodynamics of 2-(1'-Hydroxycyclohexyl)cyclohexanone: Vaporization, Sublimation, and the Ideal Gas State Thermodynamic Properties

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic Properties for 2-(1'-Hydroxycyclohexyl)cyclohexanone	https://www.doi.org/10.1021/je0501078
Thermodynamic Properties of Dimerization of 2-(1'-Hydroxycyclohexyl)cyclohexanone	https://www.doi.org/10.1021/je0602768
Vaporization, Sublimation, and the Ideal Gas State Thermodynamic Properties	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=C28746998&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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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