

cis-4-Hydroxycyclohexanecarboxylic acid lactone

Other names:	2-Oxabicyclo[2,2,2]octan-3-one 2-Oxabicyclo[2.2.2]octan-3-one
Inchi:	InChI=1S/C7H10O2/c8-7-5-1-3-6(9-7)4-2-5/h5-6H,1-4H2
InchiKey:	NVORRKXXHHFWDH-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	O=C1OC2CCCC1CC2
Mol. weight [g/mol]:	126.15
CAS:	4350-84-9

Physical Properties

Property code	Value	Unit	Source
chs	-3717.50 ± 1.30	kJ/mol	NIST Webbook
gf	-103.35	kJ/mol	Joback Method
hf	-396.60 ± 2.60	kJ/mol	NIST Webbook
hfs	-466.20 ± 1.60	kJ/mol	NIST Webbook
hfus	13.44	kJ/mol	Joback Method
hsub	69.60 ± 2.10	kJ/mol	NIST Webbook
hsub	69.60	kJ/mol	NIST Webbook
hvap	40.10	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.102		Crippen Method
mcvol	95.210	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	476.35	K	Joback Method
tc	708.35	K	Joback Method
tf	292.28	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.43	J/mol×K	476.35	Joback Method
cpg	235.02	J/mol×K	515.02	Joback Method
cpg	249.68	J/mol×K	553.68	Joback Method

cpg	263.44	J/mol×K	592.35	Joback Method
cpg	276.35	J/mol×K	631.01	Joback Method
cpg	288.42	J/mol×K	669.68	Joback Method
cpg	299.70	J/mol×K	708.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4350849&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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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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