Cyclohexanone, 2-hydroxy-

Other names:	Adipoin
	2-Hydroxycyclohexanone
	2-Hydroxy-1-cyclohexanone
	2-hydroxycyclohexan-1-one
Inchi:	InChI=1S/C6H10O2/c7-5-3-1-2-4-6(5)8/h5,7H,1-4H2
InchiKey:	ODZTXUXIYGJLMC-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	O=C1CCCCC1O
Mol. weight [g/mol]:	114.14
CAS:	533-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-235.32	kJ/mol	Joback Method
hf	-402.78	kJ/mol	Joback Method
hfus	6.73	kJ/mol	Joback Method
hvap	50.30	kJ/mol	Joback Method
ie	9.70	eV	NIST Webbook
log10ws	-0.88		Crippen Method
logp	0.490		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
rinpol	955.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	955.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1643.00		NIST Webbook
tb	516.23	K	Joback Method
tc	727.75	K	Joback Method
tf	383.00 ± 4.00	K	NIST Webbook
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.57	J/mol×K	516.23	Joback Method
cpg	225.96	J/mol×K	551.48	Joback Method
cpg	237.79	J/mol×K	586.74	Joback Method
cpg	249.05	J/mol×K	621.99	Joback Method
cpg	259.74	J/mol×K	657.24	Joback Method
cpg	269.84	J/mol×K	692.49	Joback Method
cpg	279.34	J/mol×K	727.75	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=C533608&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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