2-Hydroxy-3-methyl-2-cyclohexen-1-one

Inchi: InChI=1S/C7H10O2/c1-5-3-2-4-6(8)7(5)9/h9H,2-4H2,1H3
InchiKey: JVQYXBKQKZPLBC-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1=C(O)C(=O)CCC1
Mol. weight [g/mol]: 126.15

Physical Properties

Property code	Value	Unit	Source
gf	-208.49	kJ/mol	Joback Method
hf	-368.24	kJ/mol	Joback Method
hfus	8.69	kJ/mol	Joback Method
hvap	54.46	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.571		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
ripol	1793.00		NIST Webbook
ripol	1794.00		NIST Webbook
ripol	1794.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1793.00		NIST Webbook
tb	552.90	K	Joback Method
tc	765.39	K	Joback Method
tf	335.11	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.79	J/mol×K	552.90	Joback Method
cpg	248.06	J/mol×K	588.32	Joback Method
cpg	258.83	J/mol×K	623.73	Joback Method
cpg	269.08	J/mol×K	659.15	Joback Method
cpg	278.81	J/mol×K	694.56	Joback Method

cpg	287.99	J/mol×K	729.98	Joback Method
cpg	296.63	J/mol×K	765.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R533081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume