1-Hydroxy-3-methyl-2-butanone

Other names:	2-Butanone, 1-hydroxy-3-methyl-
Inchi:	InChI=1S/C5H10O2/c1-4(2)5(7)3-6/h4,6H,3H2,1-2H3
InchiKey:	NBEGXSQMVJTIAR-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC(C)C(=O)CO
Mol. weight [g/mol]:	102.13
CAS:	36960-22-2

Physical Properties

Property code	Value	Unit	Source
gf	-276.96	kJ/mol	Joback Method
hf	-416.62	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	0.204		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	459.41	K	Joback Method
tc	635.76	K	Joback Method
tf	241.86	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.94	J/mol×K	459.41	Joback Method
cpg	191.99	J/mol×K	488.80	Joback Method
cpg	199.72	J/mol×K	518.19	Joback Method
cpg	207.12	J/mol×K	547.58	Joback Method
cpg	214.20	J/mol×K	576.97	Joback Method
cpg	220.97	J/mol×K	606.37	Joback Method
cpg	227.44	J/mol×K	635.76	Joback Method
dvisc	0.0540168	Pa×s	241.86	Joback Method

dvisc	0.0120393	Pa×s	278.12	Joback Method
dvisc	0.0037936	Pa×s	314.38	Joback Method
dvisc	0.0015179	Pa×s	350.63	Joback Method
dvisc	0.0007211	Pa×s	386.89	Joback Method
dvisc	0.0003892	Pa×s	423.15	Joback Method
dvisc	0.0002315	Pa×s	459.41	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36960222&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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