1-Hydroxy-2-butanone

Other names: 2-Butanone, 1-hydroxy-
1-hydroxybutan-2-one
Inchi: InChI=1S/C4H8O2/c1-2-4(6)3-5/h5H,2-3H2,1H3
InchiKey: GFAZHVHNLUBROE-UHFFFAOYSA-N
Formula: C4H8O2
SMILES: CCC(=O)CO
Mol. weight [g/mol]: 88.11
CAS: 5077-67-8

Physical Properties

Property code	Value	Unit	Source
gf	-282.94	kJ/mol	Joback Method
hf	-390.70	kJ/mol	Joback Method
hfus	11.80	kJ/mol	Joback Method
hvap	47.92	kJ/mol	Joback Method
log10ws	-0.04		Crippen Method
logp	-0.042		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
rinpol	748.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	739.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1380.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1385.00		NIST Webbook

ripol	1394.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1353.00		NIST Webbook
tb	433.20	K	NIST Webbook
tc	610.84	K	Joback Method
tf	245.59	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.10	J/mol×K	436.97	Joback Method
cpg	176.47	J/mol×K	581.86	Joback Method
cpg	170.89	J/mol×K	552.88	Joback Method
cpg	165.07	J/mol×K	523.90	Joback Method
cpg	159.00	J/mol×K	494.93	Joback Method
cpg	152.68	J/mol×K	465.95	Joback Method
cpg	181.81	J/mol×K	610.84	Joback Method
dvisc	0.0002812	Pa×s	436.97	Joback Method
dvisc	0.0004536	Pa×s	405.07	Joback Method
dvisc	0.0007939	Pa×s	373.18	Joback Method
dvisc	0.0015427	Pa×s	341.28	Joback Method
dvisc	0.0034383	Pa×s	309.38	Joback Method
dvisc	0.0092130	Pa×s	277.49	Joback Method
dvisc	0.0318897	Pa×s	245.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.20	K	8.00	NIST Webbook

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=C5077678&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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume