2-Butanone, 4-hydroxy-

Other names:	Methylolacetone
	Monomethylolacetone
	3-Ketobutan-1-ol
	3-Oxo-1-butanol
	3-Oxobutanol
	4-Butanol-2-one
	4-Hydroxy-2-butanone
	NSC 41219
	4-hydroxybutan-2-one
Inchi:	InChI=1S/C4H8O2/c1-4(6)2-3-5/h5H,2-3H2,1H3
InchiKey:	LVSQXDHWDCMMRJ-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CC(=O)CCO
Mol. weight [g/mol]:	88.11

Physical Properties

Property code	Value	Unit	Source
af	0.6057		Cheméo Relay (1.0)
gf	-282.94	kJ/mol	Joback Method
hf	-411.94	kJ/mol	Cheméo Relay (1.0)
hfus	11.80	kJ/mol	Joback Method
hvap	55.08	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	1.14		Cheméo Relay (1.0)
logp	-0.042		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
rinpol	751.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	798.00		NIST Webbook
tb	446.40	K	Cheméo Relay (1.0)
tc	650.20	K	Cheméo Relay (1.0)
tf	226.88	K	Cheméo Relay (1.0)
vc	0.260	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.70	K	4.00	NIST Webbook
tbrp	363.20	K	1.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C590909&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume