Butanal, 3-hydroxy-

Other names:	Butyraldehyde, 3-hydroxy-
	«beta»-Hydroxybutyraldehyde
	Acetaldol
	Aldol
	3-Butanolal
	3-Hydroxybutyraldehyde
	Oxybutanal
	Oxybutyric aldehyde
	3-Hydroxybutanal
	UN 2839
	beta-Hydroxybutyraldehyde
	NSC 7610
Inchi:	InChI=1S/C4H8O2/c1-4(6)2-3-5/h3-4,6H,2H2,1H3
InchiKey:	HSJKGGMUJITCBW-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	CC(O)CC=O
Mol. weight [g/mol]:	88.11
CAS:	107-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-255.98	kJ/mol	Joback Method
hf	-368.98	kJ/mol	Joback Method
hfus	8.97	kJ/mol	Joback Method
hvap	47.51	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.044		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4903.92	kPa	Joback Method
tb	431.32	K	Joback Method
tc	604.34	K	Joback Method
tf	222.66	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.52	J/mol×K	431.32	Joback Method
cpg	178.75	J/mol×K	575.51	Joback Method
cpg	173.21	J/mol×K	546.67	Joback Method
cpg	167.43	J/mol×K	517.83	Joback Method
cpg	161.39	J/mol×K	488.99	Joback Method
cpg	155.08	J/mol×K	460.16	Joback Method
cpg	184.05	J/mol×K	604.34	Joback Method
dvisc	0.0003004	Pa×s	431.32	Joback Method
dvisc	0.0005135	Pa×s	396.54	Joback Method
dvisc	0.0009732	Pa×s	361.77	Joback Method
dvisc	0.0021130	Pa×s	326.99	Joback Method
dvisc	0.0055176	Pa×s	292.21	Joback Method
dvisc	0.0186726	Pa×s	257.44	Joback Method
dvisc	0.0924811	Pa×s	222.66	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107891&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
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