Dihydroxyacetone

Other names:	2-Propanone, 1,3-dihydroxy-
	Chromelin
	Dihyxal
	Otan
	Oxantin
	Oxatone
	Soleal
	Triulose
	Viticolor
	1,3-Dihydroxy-2-propanone
	1,3-Dihydroxyacetone
	NSC-24343
	1,3-Dihydroxypropanone
	1,3-Dihydroxydimethyl ketone
	Ketochromin
Inchi:	InChI=1S/C3H6O3/c4-1-3(6)2-5/h4-5H,1-2H2
InchiKey:	RXKJFZQQPQGTFL-UHFFFAOYSA-N
Formula:	C3H6O3
SMILES:	O=C(CO)CO
Mol. weight [g/mol]:	90.08
CAS:	96-26-4

Physical Properties

Property code	Value	Unit	Source
chs	-1436.00	kJ/mol	NIST Webbook
gf	-428.18	kJ/mol	Joback Method
hf	-522.29	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	62.38	kJ/mol	Joback Method
log10ws	1.11		Crippen Method
logp	-1.460		Crippen Method
mcvol	66.440	ml/mol	McGowan Method
pc	6308.83	kPa	Joback Method
ripol	2068.00		NIST Webbook
ripol	2075.00		NIST Webbook
ripol	2068.00		NIST Webbook
tb	506.27	K	Joback Method

tc	675.04	K	Joback Method
tf	348.00 ± 3.00	K	NIST Webbook
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.59	J/mol×K	506.27	Joback Method
cpg	147.33	J/mol×K	534.40	Joback Method
cpg	151.87	J/mol×K	562.53	Joback Method
cpg	156.21	J/mol×K	590.66	Joback Method
cpg	160.37	J/mol×K	618.78	Joback Method
cpg	164.34	J/mol×K	646.91	Joback Method
cpg	168.13	J/mol×K	675.04	Joback Method
dvisc	0.0465362	Pa×s	295.14	Joback Method
dvisc	0.0099350	Pa×s	330.33	Joback Method
dvisc	0.0028554	Pa×s	365.52	Joback Method
dvisc	0.0010216	Pa×s	400.70	Joback Method
dvisc	0.0004315	Pa×s	435.89	Joback Method
dvisc	0.0002073	Pa×s	471.08	Joback Method
dvisc	0.0001103	Pa×s	506.27	Joback Method

Sources

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=C96264&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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