

2,2-Dimethyl-3-hydroxypropionaldehyde

Other names:	3-Hydroxypivalaldehyde Hydroxypivaldehyde Propanal, 3-hydroxy-2,2-dimethyl- 3-hydroxy-2,2-dimethylpropionaldehyde
Inchi:	InChI=1S/C5H10O2/c1-5(2,3-6)4-7/h3,7H,4H2,1-2H3
InchiKey:	JJMOMMLADQPZNY-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC(C)(C=O)CO
Mol. weight [g/mol]:	102.13
CAS:	597-31-9

Physical Properties

Property code	Value	Unit	Source
gf	-242.28	kJ/mol	Joback Method
hf	-393.09	kJ/mol	Joback Method
hfus	7.67	kJ/mol	Joback Method
hvap	48.83	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	0.204		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	451.41	K	Joback Method
tc	630.01	K	Joback Method
tf	251.35	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.75	J/mol×K	451.41	Joback Method
cpg	197.18	J/mol×K	481.18	Joback Method
cpg	205.15	J/mol×K	510.94	Joback Method
cpg	212.68	J/mol×K	540.71	Joback Method
cpg	219.79	J/mol×K	570.48	Joback Method

cpg	226.50	J/mol×K	600.25	Joback Method
cpg	232.84	J/mol×K	630.01	Joback Method
dvisc	0.0496499	Pa×s	251.35	Joback Method
dvisc	0.0126525	Pa×s	284.69	Joback Method
dvisc	0.0042947	Pa×s	318.04	Joback Method
dvisc	0.0017896	Pa×s	351.38	Joback Method
dvisc	0.0008679	Pa×s	384.72	Joback Method
dvisc	0.0004724	Pa×s	418.07	Joback Method
dvisc	0.0002813	Pa×s	451.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.20	K	0.50	NIST Webbook

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=C597319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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