Dimethylolpropionic acid

Other names:	2,2-Dihydroxymethylpropanoic acid 2,2-Dimethylolpropionic acid 2,2-bis(hydroxymethyl)propanoic acid 2,2-bis(hydroxymethyl)propionic acid Hydracrylic acid, 2-(hydroxymethyl)-2-methyl- NSC 96616 Propanoic acid, 3-hydroxy-2-(hydroxymethyl)-2-methyl- Propionic acid, 2,2-bis(hydroxymethyl)- propanoic acid, 2,2-bis(hydroxymethyl)- «alpha»,«alpha»-Bis(hydroxymethyl)propionic acid «alpha»,«alpha»-Dimethylolpropionic acid
Inchi:	InChI=1S/C5H10O4/c1-5(2-6,3-7)4(8)9/h6-7H,2-3H2,1H3,(H,8,9)
InchiKey:	PTBDIHRZYDMNKB-UHFFFAOYSA-N
Formula:	C5H10O4
SMILES:	CC(CO)(CO)C(=O)O
Mol. weight [g/mol]:	134.13
CAS:	4767-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-545.32	kJ/mol	Joback Method
hf	-724.55	kJ/mol	Joback Method
hfus	38.76	kJ/mol	Thermal analysis of phase change materials in the temperature range 120.150 .C
hvap	82.21	kJ/mol	Joback Method
log10ws	0.70		Crippen Method
logp	-0.938		Crippen Method
mcvol	100.490	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
tb	640.98	K	Joback Method
tc	811.32	K	Joback Method
tf	468.70 ± 3.00	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.84	J/mol×K	669.37	Joback Method
cpg	278.58	J/mol×K	697.76	Joback Method
cpg	284.01	J/mol×K	726.15	Joback Method
cpg	298.56	J/mol×K	811.32	Joback Method
cpg	289.14	J/mol×K	754.54	Joback Method
cpg	293.98	J/mol×K	782.93	Joback Method
cpg	266.75	J/mol×K	640.98	Joback Method
dvisc	0.0000188	Pa×s	597.64	Joback Method
dvisc	0.0000436	Pa×s	554.29	Joback Method
dvisc	0.0001167	Pa×s	510.95	Joback Method
dvisc	0.0003744	Pa×s	467.61	Joback Method
dvisc	0.0015244	Pa×s	424.26	Joback Method
dvisc	0.0000091	Pa×s	640.98	Joback Method
dvisc	0.0085437	Pa×s	380.92	Joback Method
hfust	38.50	kJ/mol	426.00	NIST Webbook
hfust	3.59	kJ/mol	468.00	NIST Webbook
hfust	3.59	kJ/mol	468.00	NIST Webbook
sfust	7.68	J/mol×K	468.00	NIST Webbook
sfust	90.37	J/mol×K	426.00	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=C4767037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal analysis of phase change materials in the temperature range 120.150 .C:	https://www.doi.org/10.1016/j.tca.2010.11.011

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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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