PROPANOIC ACID, 3-HYDROXY-2-(HYDROXYMETHYL)-2-METHYL-

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
Propionic acid, 2,2-bis(hydroxymethyl)-
dimethylolpropionic acid
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

Physical Properties

Property code	Value	Unit	Source
af	0.8439		Cheméo Relay (1.0)
gf	-545.32	kJ/mol	Joback Method
hf	-778.31	kJ/mol	Cheméo Relay (1.0)
hfus	38.76	kJ/mol	Thermal analysis of phase change materials in the temperature range 120.150 .C
hvap	91.30	kJ/mol	Cheméo Relay (1.0)
ie	10.21	eV	Cheméo Relay (1.0)
log10ws	-0.05		Cheméo Relay (1.0)
logp	-0.938		Crippen Method
mcvol	100.490	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
tb	552.06	K	Cheméo Relay (1.0)
tc	794.45	K	Cheméo Relay (1.0)
tf	468.70 ± 3.00	K	NIST Webbook
vc	0.354	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.75	J/mol×K	640.98	Joback Method
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	289.14	J/mol×K	754.54	Joback Method
cpg	293.98	J/mol×K	782.93	Joback Method
cpg	298.56	J/mol×K	811.32	Joback Method
dvisc	0.0085437	Pa×s	380.92	Joback Method
dvisc	0.0015244	Pa×s	424.26	Joback Method
dvisc	0.0003744	Pa×s	467.61	Joback Method
dvisc	0.0001167	Pa×s	510.95	Joback Method
dvisc	0.0000436	Pa×s	554.29	Joback Method
dvisc	0.0000188	Pa×s	597.64	Joback Method
dvisc	0.0000091	Pa×s	640.98	Joback Method
hfust	3.59	kJ/mol	468.00	NIST Webbook
hfust	38.50	kJ/mol	426.00	NIST Webbook
hfust	3.59	kJ/mol	468.00	NIST Webbook
sfust	90.37	J/mol×K	426.00	NIST Webbook
sfust	7.68	J/mol×K	468.00	NIST Webbook

Sources

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):

Cheméo Relay (1.0, beta):

Thermal analysis of phase change materials in the temperature range 120.150 °C: https://www.doi.org/10.1016/j.tca.2010.11.011

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4767037&Units=SI

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

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

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