

Hydroxypivalic acid

Other names:	Propanoic acid, 3-hydroxy-2,2-dimethyl- 2,2-Dimethyl-3-hydroxypropionic acid 3-hydroxypivalic acid
Inchi:	InChI=1S/C5H10O3/c1-5(2,3-6)4(7)8/h6H,3H2,1-2H3,(H,7,8)
InchiKey:	RDFQSFOGKVZWKF-UHFFFAOYSA-N
Formula:	C5H10O3
SMILES:	CC(C)(CO)C(=O)O
Mol. weight [g/mol]:	118.13
CAS:	4835-90-9

Physical Properties

Property code	Value	Unit	Source
gf	-408.50	kJ/mol	Joback Method
hf	-572.32	kJ/mol	Joback Method
hfus	11.07	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-0.04		Crippen Method
logp	0.089		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
tb	548.80	K	Joback Method
tc	724.01	K	Joback Method
tf	320.10	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.03	J/molxK	548.80	Joback Method
cpg	235.28	J/molxK	578.00	Joback Method
cpg	242.14	J/molxK	607.20	Joback Method
cpg	248.61	J/molxK	636.41	Joback Method
cpg	254.72	J/molxK	665.61	Joback Method
cpg	260.49	J/molxK	694.81	Joback Method

cpg	265.93	J/mol×K	724.01	Joback Method
dvisc	0.0296306	Paxs	320.10	Joback Method
dvisc	0.0061970	Paxs	358.22	Joback Method
dvisc	0.0017512	Paxs	396.33	Joback Method
dvisc	0.0006177	Paxs	434.45	Joback Method
dvisc	0.0002578	Paxs	472.57	Joback Method
dvisc	0.0001226	Paxs	510.68	Joback Method
dvisc	0.0000646	Paxs	548.80	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=C4835909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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