1,3-Benzenedimethanol, 2-hydroxy-5-methyl-

Other names:	«alpha»1,«alpha»3-Mesitylenediol, 2-hydroxy- «alpha»1,«alpha»3, 2-Trihydroxymesitylene 2,6-Bis(hydroxymethyl)-p-cresol 2,6-Bis(hydroxymethyl)-4-methylphenol 2,6-Di(hydroxymethyl)-p-cresol 2,6-Dimethylol-p-cresol 2,6-Dimethylol-4-methylphenol 2-Hydroxy-5-methyl-1,3-benzenedimethanol 4-Methyl-2,6-bis(hydroxymethyl)-phenol NSC 15838 A^1,a^3-mesityllenediol, 2-hydroxy- 3,5-bis(hydroxymethyl)-p-cresol A
Inchi:	InChI=1S/C9H12O3/c1-6-2-7(4-10)9(12)8(3-6)5-11/h2-3,10-12H,4-5H2,1H3
InchiKey:	KUMMBDBTERQYCG-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	Cc1cc(CO)c(O)c(CO)c1
Mol. weight [g/mol]:	168.19
CAS:	91-04-3

Physical Properties

Property code	Value	Unit	Source
gf	-310.21	kJ/mol	Joback Method
hf	-497.27	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	85.60	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	0.685		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	706.94	K	Joback Method
tc	903.26	K	Joback Method
tf	476.01	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.02	J/mol×K	706.94	Joback Method
cpg	363.26	J/mol×K	739.66	Joback Method
cpg	371.11	J/mol×K	772.38	Joback Method
cpg	378.62	J/mol×K	805.10	Joback Method
cpg	385.83	J/mol×K	837.82	Joback Method
cpg	392.79	J/mol×K	870.54	Joback Method
cpg	399.55	J/mol×K	903.26	Joback Method
dvisc	0.0001866	Pa×s	476.01	Joback Method
dvisc	0.0000617	Pa×s	514.50	Joback Method
dvisc	0.0000238	Pa×s	552.99	Joback Method
dvisc	0.0000104	Pa×s	591.48	Joback Method
dvisc	0.0000050	Pa×s	629.96	Joback Method
dvisc	0.0000026	Pa×s	668.45	Joback Method
dvisc	0.0000015	Pa×s	706.94	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=C91043&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume