2,4,6-Trihydroxytoluene

Other names: 1,3,5-Benzenetriol, 2-methyl-
Methylphloroglucinol
Phloroglucinol, methyl-
Toluene-2,4,6-triol
2-Methylphloroglucinol
2-Methyl-1,3,5-benzenetriol
Inchi: InChI=1S/C7H8O3/c1-4-6(9)2-5(8)3-7(4)10/h2-3,8-10H,1H3
InchiKey: BPHYZRNTQNPLFI-UHFFFAOYSA-N
Formula: C7H8O3
SMILES: Cc1c(O)cc(O)cc1O
Mol. weight [g/mol]: 140.14
CAS: 88-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-343.39	kJ/mol	Joback Method
hf	-483.21	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	72.49	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	1.112		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	8087.06	kPa	Joback Method
tb	628.10	K	Joback Method
tc	881.41	K	Joback Method
tf	530.23	K	Joback Method
vc	0.217	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.27	J/mol×K	628.10	Joback Method
cpg	298.79	J/mol×K	839.19	Joback Method
cpg	292.12	J/mol×K	796.97	Joback Method

cpg	285.55	J/mol×K	754.76	Joback Method
cpg	278.87	J/mol×K	712.54	Joback Method
cpg	271.85	J/mol×K	670.32	Joback Method
cpg	305.80	J/mol×K	881.41	Joback Method
dvisc	0.0000008	Pa×s	628.10	Joback Method
dvisc	0.0000011	Pa×s	611.79	Joback Method
dvisc	0.0000016	Pa×s	595.48	Joback Method
dvisc	0.0000024	Pa×s	579.16	Joback Method
dvisc	0.0000037	Pa×s	562.85	Joback Method
dvisc	0.0000059	Pa×s	546.54	Joback Method
dvisc	0.0000095	Pa×s	530.23	Joback Method

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=C88039&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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