1,3,5-Benzenetriol

Other names:	Phloroglucinol
	s-Trihydroxybenzene
	Benzene-s-triol
	Phloroglucin
	Phloroglucine
	1,3,5-Trihydroxybenzene
	sym-Trihydroxybenzene
	Benzene, trihydroxy
	Benzene, 1,3,5-trihydroxy-
	Spasfon-Lyoc
	1,3,5-Trihydroxycyclohexatriene
	3,5-Dihydroxyphenol
	5-Hydroxyresorcinol
	5-Oxyresorcinolphloroglucin
	Benzene-1,3,5-triol
	Dilospan S
	Floroglucin
	Floroglucinol
	5-Oxyresorcinol
	1,3,5-THB
	NSC 1572
	Phloroglucinol (1,3,5-benzenetriol)
Inchi:	InChI=1S/C6H6O3/c7-4-1-5(8)3-6(9)2-4/h1-3,7-9H
InchiKey:	QCDYQQDYXPDABM-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	Oc1cc(O)cc(O)c1
Mol. weight [g/mol]:	126.11
CAS:	108-73-6

Physical Properties

Property code	Value	Unit	Source
chs	-2634.00 ± 0.70	kJ/mol	NIST Webbook
gf	-342.18	kJ/mol	Joback Method
hf	-452.90 ± 1.50	kJ/mol	NIST Webbook
hfs	-584.60 ± 1.10	kJ/mol	NIST Webbook
hfus	23.07	kJ/mol	Joback Method

hsub	131.70 ± 1.00	kJ/mol	NIST Webbook
hsub	135.50 ± 1.30	kJ/mol	NIST Webbook
hsub	131.70	kJ/mol	NIST Webbook
hsub	131.70 ± 1.00	kJ/mol	NIST Webbook
hvap	69.61	kJ/mol	Joback Method
log10ws	-0.12		Crippen Method
logp	0.803		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	9980.03	kPa	Joback Method
rinpol	1609.60		NIST Webbook
tb	600.24	K	Joback Method
tc	858.52	K	Joback Method
tf	506.44	K	Joback Method
vc	0.162	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.40	J/mol×K	600.24	Joback Method
cpg	229.07	J/mol×K	643.29	Joback Method
cpg	235.05	J/mol×K	686.33	Joback Method
cpg	240.59	J/mol×K	729.38	Joback Method
cpg	245.92	J/mol×K	772.43	Joback Method
cpg	251.30	J/mol×K	815.47	Joback Method
cpg	256.97	J/mol×K	858.52	Joback Method
dvisc	0.0000112	Pa×s	522.07	Joback Method
dvisc	0.0000185	Pa×s	506.44	Joback Method
dvisc	0.0000070	Pa×s	537.71	Joback Method
dvisc	0.0000045	Pa×s	553.34	Joback Method
dvisc	0.0000029	Pa×s	568.97	Joback Method
dvisc	0.0000020	Pa×s	584.61	Joback Method
dvisc	0.0000013	Pa×s	600.24	Joback Method
hfust	34.50	kJ/mol	491.80	NIST Webbook
hsubt	127.90	kJ/mol	394.50	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=C108736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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