

1,2,4-Benzenetriol

Other names:	1,3,4-Benzenetriol
	2,5-Dihydroxyphenol
	Hydroxyhydroquinone
	2-Hydroxy-1,4-hydroquinone
	1,2,4-Trihydroxybenzene
	1,3,4-Trihydroxybenzene
	Benzene-1,2,4-triol
	Hydroquinone, hydroxy-
	Hydroxyquinol
	Oxyhydrochinon
	Oxyhydroquinone
	NSC 2818
	2-Hydroxy-p-benzohydroquinone
Inchi:	InChI=1S/C6H6O3/c7-4-1-2-5(8)6(9)3-4/h1-3,7-9H
InchiKey:	GGNQARNBDZQJCCN-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	Oc1ccc(O)c(O)c1
Mol. weight [g/mol]:	126.11
CAS:	533-73-3

Physical Properties

Property code	Value	Unit	Source
chs	-2654.80 ± 0.80	kJ/mol	NIST Webbook
gf	-342.18	kJ/mol	Joback Method
hf	-444.00 ± 1.60	kJ/mol	NIST Webbook
hfs	-563.80 ± 1.10	kJ/mol	NIST Webbook
hfus	23.07	kJ/mol	Joback Method
hsub	119.80 ± 1.60	kJ/mol	NIST Webbook
hsub	124.20 ± 0.60	kJ/mol	NIST Webbook
hsub	119.80	kJ/mol	NIST Webbook
hsub	119.80 ± 1.20	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
tb	600.24	K	Joback Method

tc	858.52	K	Joback Method
tf	506.44	K	Joback Method
vc	0.162	m ³ /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	0.0000185	Pa×s	506.44	Joback Method
dvisc	0.0000112	Pa×s	522.07	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	28.80	kJ/mol	413.20	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=C533733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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

Latest version available from:

<https://www.cheméo.com/cid/37-376-4/1-2-4-Benzenetriol.pdf>

Generated by Cheméo on 2025-12-24 08:26:03.955929387 +0000 UTC m=+6312961.485970054.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.