1,4-Benzenediol, 2-methyl-

Other names:	1,4-dihydroxy-2-methylbenzene
	2,5-Dihydroxytoluene
	2,5-toluenediol
	2-Methyl-1,4-benzenediol (2-methylhydroquinone)
	2-Methyl-1,4-hydroquinone
	2-Methyl-p-hydroquinone
	2-methyl-1,4-benzenediol
	2-methylhydroquinone
	Methyl-p-hydroquinone
	Methylhydroquinone
	NSC 4962
	THQ
	Toluhydroquinone
	Tolylhydroquinone
	hydroquinone, methyl-
	p-Toluhydroquinone
	p-Toluquinol
	p-toluhydroquinol
	toluquinol
Inchi:	InChI=1S/C7H8O2/c1-5-4-6(8)2-3-7(5)9/h2-4,8-9H,1H3
InchiKey:	CNHDIAIOKMXOLK-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	Cc1cc(O)ccc1O
Mol. weight [g/mol]:	124.14
CAS:	95-71-6

Physical Properties

Property code	Value	Unit	Source
chs	-3492.00	kJ/mol	NIST Webbook
gf	-188.77	kJ/mol	Joback Method
hf	-305.90	kJ/mol	Joback Method
hfus	19.49	kJ/mol	Joback Method
hsub	100.40 ± 1.40	kJ/mol	NIST Webbook
hsub	108.40 ± 3.90	kJ/mol	NIST Webbook
hvap	59.48	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.406		Crippen Method

mcvol	97.470	ml/mol	McGowan Method
pc	6288.83	kPa	Joback Method
rinpol	1226.00		NIST Webbook
rinpol	1223.00		NIST Webbook
tb	547.48	K	Joback Method
tc	790.85	K	Joback Method
tf	418.51	K	Joback Method
vc	0.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.32	J/mol×K	790.85	Joback Method
cpg	235.94	J/mol×K	588.04	Joback Method
cpg	244.34	J/mol×K	628.60	Joback Method
cpg	252.03	J/mol×K	669.16	Joback Method
cpg	259.16	J/mol×K	709.73	Joback Method
cpg	265.88	J/mol×K	750.29	Joback Method
cpg	226.69	J/mol×K	547.48	Joback Method
cps	174.90	J/mol×K	323.00	NIST Webbook
dvisc	0.0000240	Pa×s	525.99	Joback Method
dvisc	0.0000392	Pa×s	504.49	Joback Method
dvisc	0.0000667	Pa×s	483.00	Joback Method
dvisc	0.0001192	Pa×s	461.50	Joback Method
dvisc	0.0002256	Pa×s	440.00	Joback Method
dvisc	0.0000153	Pa×s	547.48	Joback Method
dvisc	0.0004561	Pa×s	418.51	Joback Method
hfust	27.60	kJ/mol	404.20	NIST Webbook
hsubt	97.20 ± 1.40	kJ/mol	350.50	NIST Webbook
hsubt	107.80 ± 1.10	kJ/mol	333.00	NIST Webbook
psub	1.73e-04	kPa	327.15	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.98e-04	kPa	331.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	2.92e-04	kPa	331.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.77e-04	kPa	331.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.82e-04	kPa	327.15	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.61e-04	kPa	333.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.48e-04	kPa	333.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.81e-04	kPa	335.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.62e-04	kPa	335.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.48e-04	kPa	335.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	6.10e-04	kPa	337.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	6.07e-04	kPa	337.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	5.69e-04	kPa	337.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.51e-04	kPa	339.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.31e-04	kPa	339.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.04e-04	kPa	339.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	9.57e-04	kPa	341.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	9.16e-04	kPa	341.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	8.90e-04	kPa	341.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	1.89e-04	kPa	327.15	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.38e-04	kPa	325.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.44e-04	kPa	325.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.47e-04	kPa	325.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.26e-04	kPa	329.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.29e-04	kPa	329.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.39e-04	kPa	329.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.75e-04	kPa	333.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

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=C95716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental standard molar enthalpies of formation of some methylbenzenediol isomers:	https://www.doi.org/10.1016/j.jct.2009.04.015

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume