1,2-Benzenediol, 4-methyl-

Other names:	4-Methylcatechol
	3,4-Dihydroxytoluene
	Homocatechol
	Homopyrocatechol
	2-Hydroxy-4-methylphenol
	4-Methyl-1,2-benzenediol
	4-Methyl-1,2-dihydroxybenzene
	p-Methylpyrocatechol
	4-Methylpyrocatechol
	Pyrocatechol, 4-methyl-
	Toluene-3,4-diol
	1,2-Dihydroxy-4-methylbenzene
	4-Methylbenzene-1,2-diol
	1-Methyl-3,4-dihydroxybenzene
	NSC 17489
	p-Methylcatechol
	4-Methyl-1,2-benzenediol (4-methylpyrocatechol)
Inchi:	InChI=1S/C7H8O2/c1-5-2-3-6(8)7(9)4-5/h2-4,8-9H,1H3
InchiKey:	ZBCATMYQYDCTIZ-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	Cc1ccc(O)c(O)c1
Mol. weight [g/mol]:	124.14
CAS:	452-86-8

Physical Properties

Property code	Value	Unit	Source
chs	-3504.60 ± 0.60	kJ/mol	NIST Webbook
gf	-188.77	kJ/mol	Joback Method
hf	-298.40 ± 1.60	kJ/mol	NIST Webbook
hfs	-393.30 ± 1.20	kJ/mol	NIST Webbook
hfus	19.49	kJ/mol	Joback Method
hsub	94.90 ± 1.00	kJ/mol	NIST Webbook
hsub	94.90 ± 1.00	kJ/mol	NIST Webbook
hsub	94.90	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	1293.60		NIST Webbook
rinpol	1295.10		NIST Webbook
rinpol	1293.00		NIST Webbook
ripol	2727.00		NIST Webbook
ripol	2727.00		NIST Webbook
tb	524.20	K	NIST Webbook
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	226.69	J/mol×K	547.48	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	272.32	J/mol×K	790.85	Joback Method
dvisc	0.0004561	Pa×s	418.51	Joback Method
dvisc	0.0002256	Pa×s	440.00	Joback Method
dvisc	0.0001192	Pa×s	461.50	Joback Method
dvisc	0.0000667	Pa×s	483.00	Joback Method
dvisc	0.0000392	Pa×s	504.49	Joback Method
dvisc	0.0000240	Pa×s	525.99	Joback Method
dvisc	0.0000153	Pa×s	547.48	Joback Method
hvapt	90.00	kJ/mol	401.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C452868&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume