1,3-benzenediol, 4-methyl-

Other names:	1,3-dihydroxy-4-methylbenzene
	2,4-toluenediol
	4-methyl-1,3-benzenediol
	4-methylresorcinol
	cresorcinol
	resorcinol, 4-methyl-
Inchi:	InChI=1S/C7H8O2/c1-5-2-3-6(8)4-7(5)9/h2-4,8-9H,1H3
InchiKey:	FNYDIAAMUCQQDE-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	Cc1ccc(O)cc1O
Mol. weight [g/mol]:	124.14

Physical Properties

Property code	Value	Unit	Source
gf	-188.77	kJ/mol	Joback Method
hf	-305.90	kJ/mol	Joback Method
hfus	19.49	kJ/mol	Joback Method
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
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
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
psub	2.15e-04	kPa	321.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.11e-04	kPa	321.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.82e-04	kPa	323.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.66e-04	kPa	323.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.62e-04	kPa	323.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.61e-04	kPa	325.23	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.20e-04	kPa	321.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	3.36e-04	kPa	325.23	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.51e-04	kPa	327.13	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.38e-04	kPa	327.13	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.32e-04	kPa	327.13	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	5.72e-04	kPa	329.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	5.62e-04	kPa	329.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	5.61e-04	kPa	329.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.42e-04	kPa	331.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	7.24e-04	kPa	331.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.19e-04	kPa	331.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	9.33e-04	kPa	333.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	9.16e-04	kPa	333.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	8.86e-04	kPa	333.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.66e-04	kPa	319.22	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.70e-04	kPa	319.22	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.75e-04	kPa	319.22	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.28e-04	kPa	317.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	1.29e-04	kPa	317.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.34e-04	kPa	317.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.44e-04	kPa	325.23	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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