Orcinol

Other names:	1,3-benzenediol, 5-methyl-
	1,3-dihydroxy-5-methylbenzene
	3,5-Dihydroxytoluene
	3,5-Toluenediol
	3-Hydroxy-5-methylphenol
	5-Methyl-1,3-dihydroxybenzene
	5-Methylresorcin
	5-Methylresorcinol
	5-methyl-1,3-benzenediol
	Dihydroxytoluene
	Methylresorcinol
	NSC 12441
	Orcine
	orcin
	resorcinol, 5-methyl-
Inchi:	InChI=1S/C7H8O2/c1-5-2-6(8)4-7(9)3-5/h2-4,8-9H,1H3
InchiKey:	OIPPWFOQEKKFEE-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	Cc1cc(O)cc(O)c1
Mol. weight [g/mol]:	124.14
CAS:	504-15-4

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
hsub	102.90 ± 3.50	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	1369.00		NIST Webbook
rinpol	1378.10		NIST Webbook
tb	562.70	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	252.03	J/mol×K	669.16	Joback Method
cpg	235.94	J/mol×K	588.04	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
cpg	244.34	J/mol×K	628.60	Joback Method
cpg	226.69	J/mol×K	547.48	Joback Method
dvisc	0.0004561	Pa×s	418.51	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
dvisc	0.0002256	Pa×s	440.00	Joback Method
hsubt	102.30 ± 0.70	kJ/mol	330.00	NIST Webbook
hvapt	76.60	kJ/mol	435.00	NIST Webbook
psub	5.91e-04	kPa	334.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.85e-04	kPa	332.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.82e-04	kPa	332.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	6.07e-04	kPa	334.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	5.96e-04	kPa	334.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.99e-04	kPa	332.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.66e-04	kPa	336.13	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.54e-04	kPa	336.13	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.34e-04	kPa	336.13	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	9.74e-04	kPa	338.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	9.35e-04	kPa	338.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	9.32e-04	kPa	338.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	3.78e-04	kPa	330.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	
psub	3.83e-04	kPa	330.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	
psub	3.94e-04	kPa	330.14	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	
psub	3.04e-04	kPa	328.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	
psub	3.03e-04	kPa	328.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	
psub	3.11e-04	kPa	328.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	
psub	2.45e-04	kPa	326.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	
psub	2.46e-04	kPa	326.10	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers	

psub	1.93e-04	kPa	324.16	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.96e-04	kPa	324.16	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.53e-04	kPa	322.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.53e-04	kPa	322.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.57e-04	kPa	322.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.99e-04	kPa	324.16	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=C504154&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

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume