2,6-DIHYDROXYTOLUENE

Other names:	1,3-dihydroxy-2-methylbenzene
	2-Methylresorcin
	2-methylresorcinol
	Toluene-2,6-diol
	resorcinol, 2-methyl-
Inchi:	InChI=1S/C7H8O2/c1-5-6(8)3-2-4-7(5)9/h2-4,8-9H,1H3
InchiKey:	ZTMADXFOCUXMJE-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	Cc1c(O)cccc1O
Mol. weight [g/mol]:	124.14

Physical Properties

Property code	Value	Unit	Source
af	0.5969		Cheméo Relay (1.0)
gf	-188.77	kJ/mol	Joback Method
hf	-301.29	kJ/mol	Cheméo Relay (1.0)
hfus	19.49	kJ/mol	Joback Method
hsub	99.20 ± 2.30	kJ/mol	NIST Webbook
hvap	74.01	kJ/mol	Cheméo Relay (1.0)
ie	8.25	eV	Cheméo Relay (1.0)
log10ws	-0.93		Cheméo Relay (1.0)
logp	1.406		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
pc	6288.83	kPa	Joback Method
tb	537.20	K	NIST Webbook
tc	751.88	K	Cheméo Relay (1.0)
tf	396.34	K	Cheméo Relay (1.0)
vc	0.324	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.34	J/mol×K	628.60	Joback Method
cpg	259.16	J/mol×K	709.73	Joback Method

cpg	226.69	J/mol×K	547.48	Joback Method
cpg	235.94	J/mol×K	588.04	Joback Method
cpg	252.03	J/mol×K	669.16	Joback Method
cpg	272.32	J/mol×K	790.85	Joback Method
cpg	265.88	J/mol×K	750.29	Joback Method
dvisc	0.0000153	Pa×s	547.48	Joback Method
dvisc	0.0001192	Pa×s	461.50	Joback Method
dvisc	0.0004561	Pa×s	418.51	Joback Method
dvisc	0.0002256	Pa×s	440.01	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
hsubt	98.80 ± 0.30	kJ/mol	319.00	NIST Webbook
hvapt	66.90	kJ/mol	416.00	NIST Webbook
psub	2.87e-04	kPa	317.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.50e-04	kPa	319.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.56e-04	kPa	321.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.46e-04	kPa	321.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	4.37e-04	kPa	321.19	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	5.78e-04	kPa	323.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	5.59e-04	kPa	323.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	5.53e-04	kPa	323.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	7.24e-04	kPa	325.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	6.94e-04	kPa	325.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	6.73e-04	kPa	325.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	8.96e-04	kPa	327.17	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	8.83e-04	kPa	327.17	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	8.51e-04	kPa	327.17	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.12e-03	kPa	329.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	1.10e-03	kPa	329.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.08e-03	kPa	329.11	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.41e-04	kPa	319.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	3.58e-04	kPa	319.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.76e-04	kPa	317.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.80e-04	kPa	317.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.09e-04	kPa	309.22	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.17e-04	kPa	315.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	2.24e-04	kPa	315.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	2.27e-04	kPa	315.21	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.71e-04	kPa	313.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.72e-04	kPa	313.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.76e-04	kPa	313.12	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.32e-04	kPa	311.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.36e-04	kPa	311.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.41e-04	kPa	311.20	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers
psub	1.03e-04	kPa	309.22	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

psub	1.07e-04	kPa	309.22	Experimental standard molar enthalpies of formation of some methylbenzenediol isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.20	K	2.10	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Experimental standard molar enthalpies of formation of some methylbenzenediol isomers:	https://www.doi.org/10.1016/j.jct.2009.04.015
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608253&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume