

1,4-Benzenediol, 2,5-dimethyl-

Other names:	Phen-1,4-diol, 3,6-dimethyl- 2,5-dimethylhydroquinone p-Xylohydroquinone
Inchi:	InChI=1S/C8H10O2/c1-5-3-8(10)6(2)4-7(5)9/h3-4,9-10H,1-2H3
InchiKey:	GPASWZHHWPVSRG-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	<chem>Cc1cc(O)c(C)cc1O</chem>
Mol. weight [g/mol]:	138.16
CAS:	615-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-189.98	kJ/mol	Joback Method
hf	-338.01	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hsub	100.80	kJ/mol	NIST Webbook
hvap	62.37	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.715		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	5312.41	kPa	Joback Method
tb	575.34	K	Joback Method
tc	814.79	K	Joback Method
tf	442.30	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.68	J/molxK	575.34	Joback Method
cpg	278.66	J/molxK	615.25	Joback Method
cpg	287.88	J/molxK	655.16	Joback Method
cpg	296.46	J/molxK	695.07	Joback Method
cpg	304.55	J/molxK	734.98	Joback Method

cpg	312.26	J/molxK	774.89	Joback Method
cpg	319.75	J/molxK	814.79	Joback Method
dvisc	0.0001205	Paxs	464.47	Joback Method
dvisc	0.0002320	Paxs	442.30	Joback Method
dvisc	0.0000664	Paxs	486.65	Joback Method
dvisc	0.0000386	Paxs	508.82	Joback Method
dvisc	0.0000234	Paxs	530.99	Joback Method
dvisc	0.0000148	Paxs	553.17	Joback Method
dvisc	0.0000097	Paxs	575.34	Joback Method
hsubt	100.80	kJ/mol	346.50	NIST Webbook
hvapt	101.10	kJ/mol	346.00	NIST Webbook

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=C615907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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