

PHEN-1,4-DIOL, 3,6-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:	Cc1cc(O)c(C)cc1O
Mol. weight [g/mol]:	138.17

Physical Properties

Property code	Value	Unit	Source
af	0.6219		Cheméo Relay (1.0)
gf	-189.98	kJ/mol	Joback Method
hf	-326.99	kJ/mol	Cheméo Relay (1.0)
hfus	21.69	kJ/mol	Joback Method
hsub	100.80	kJ/mol	NIST Webbook
hvap	92.85	kJ/mol	Cheméo Relay (1.0)
ie	8.06	eV	Cheméo Relay (1.0)
log10ws	-1.27		Cheméo Relay (1.0)
logp	1.715		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	5312.41	kPa	Joback Method
tb	526.25	K	Cheméo Relay (1.0)
tc	757.95	K	Cheméo Relay (1.0)
tf	438.47	K	Cheméo Relay (1.0)
vc	0.390	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.75	J/mol×K	814.79	Joback Method
cpg	304.55	J/mol×K	734.98	Joback Method
cpg	268.68	J/mol×K	575.34	Joback Method
cpg	278.66	J/mol×K	615.25	Joback Method

cpg	287.88	J/mol×K	655.16	Joback Method
cpg	296.46	J/mol×K	695.07	Joback Method
cpg	312.26	J/mol×K	774.89	Joback Method
dvisc	0.0002320	Pa×s	442.30	Joback Method
dvisc	0.0001205	Pa×s	464.47	Joback Method
dvisc	0.0000664	Pa×s	486.65	Joback Method
dvisc	0.0000386	Pa×s	508.82	Joback Method
dvisc	0.0000234	Pa×s	530.99	Joback Method
dvisc	0.0000148	Pa×s	553.17	Joback Method
dvisc	0.0000097	Pa×s	575.34	Joback Method
hsubt	100.80	kJ/mol	346.50	NIST Webbook
hvapt	101.10	kJ/mol	346.00	NIST Webbook

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615907&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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