PHENOL, 4-PHENOXY-

Other names:	Phenol, p-phenoxy-
	p-Hydroxydiphenyl ether
	p-Phenoxyphenol
	4-Hydroxydiphenyl ether
	4-Phenoxyphenol
Inchi:	InChI=1S/C12H10O2/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9,13H
InchiKey:	ZSBDGXGICLIJGD-UHFFFAOYSA-N
Formula:	C12H10O2
SMILES:	Oc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	186.21

Physical Properties

Property code	Value	Unit	Source
af	0.6168		Cheméo Relay (1.0)
gf	15.36	kJ/mol	Joback Method
hf	-104.81	kJ/mol	Cheméo Relay (1.0)
hfus	21.89	kJ/mol	Joback Method
hvap	89.69	kJ/mol	Cheméo Relay (1.0)
ie	7.82	eV	Cheméo Relay (1.0)
log10ws	-2.78		Cheméo Relay (1.0)
logp	3.184		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	294.30		NIST Webbook
rinpol	294.30		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	594.96	K	Cheméo Relay (1.0)
tc	856.81	K	Cheméo Relay (1.0)
tf	375.30	K	Cheméo Relay (1.0)
vc	0.518	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.76	J/mol×K	630.36	Joback Method
cpg	366.38	J/mol×K	673.03	Joback Method
cpg	378.88	J/mol×K	715.69	Joback Method
cpg	390.37	J/mol×K	758.36	Joback Method
cpg	400.97	J/mol×K	801.02	Joback Method
cpg	410.81	J/mol×K	843.69	Joback Method
cpg	420.01	J/mol×K	886.36	Joback Method
dvisc	0.0007478	Pa×s	411.79	Joback Method
dvisc	0.0003302	Pa×s	448.22	Joback Method
dvisc	0.0001648	Pa×s	484.65	Joback Method
dvisc	0.0000907	Pa×s	521.08	Joback Method
dvisc	0.0000540	Pa×s	557.50	Joback Method
dvisc	0.0000342	Pa×s	593.93	Joback Method
dvisc	0.0000229	Pa×s	630.36	Joback Method

Sources

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=C831823&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume