

4-Phenylpyrocatechol

Other names:	[1,1'-Biphenyl]-3,4-diol 1,2-Benzenediol, 4-phenyl- 3,4-Biphenyldiol 3,4-Dihydroxybiphenyl 4-Phenyl-1,2-benzenediol 4-Phenylcatechol Biphenyl, 3,4-dihydroxy biphenyl-3,4-diol
Inchi:	InChI=1S/C12H10O2/c13-11-7-6-10(8-12(11)14)9-4-2-1-3-5-9/h1-8,13-14H
InchiKey:	QDNPCYCBQFHNJC-UHFFFAOYSA-N
Formula:	C12H10O2
SMILES:	Oc1ccc(-c2ccccc2)cc1O
Mol. weight [g/mol]:	186.21
CAS:	92-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-34.26	kJ/mol	Joback Method
hf	-172.57	kJ/mol	Joback Method
hfus	26.48	kJ/mol	Joback Method
hvap	72.89	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.765		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
rinpol	1918.00		NIST Webbook
tb	688.56	K	Joback Method
tc	956.80	K	Joback Method
tf	412.50 ± 0.50	K	NIST Webbook
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	373.78	J/molxK	688.56	Joback Method
cpg	385.57	J/molxK	733.27	Joback Method
cpg	396.50	J/molxK	777.97	Joback Method
cpg	406.80	J/molxK	822.68	Joback Method
cpg	416.72	J/molxK	867.39	Joback Method
cpg	426.49	J/molxK	912.09	Joback Method
cpg	436.36	J/molxK	956.80	Joback Method
dvisc	0.0000720	Paxs	501.28	Joback Method
dvisc	0.0000335	Paxs	532.49	Joback Method
dvisc	0.0000170	Paxs	563.71	Joback Method
dvisc	0.0000093	Paxs	594.92	Joback Method
dvisc	0.0000054	Paxs	626.13	Joback Method
dvisc	0.0000033	Paxs	657.35	Joback Method
dvisc	0.0000021	Paxs	688.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	477.00 ± 1.00	K	1.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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