

Phosphonic acid, (4-hydroxyphenyl)-

Other names:	4-Hydroxybenzenephosphonic acid (p-Hydroxyphenyl)phosphonic acid 4-Hydroxyphenylphosphonic acid Phosphonic acid, (4-hydroxyphenyl)-
Inchi:	InChI=1S/C6H7O4P/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4,7H,(H2,8,9,10)
InchiKey:	YIDVLWDHYNWHMH-UHFFFAOYSA-N
Formula:	C6H7O4P
SMILES:	O=P(O)(O)c1ccc(O)cc1
Mol. weight [g/mol]:	174.09

Physical Properties

Property code	Value	Unit	Source
hf	-634.64	kJ/mol	Cheméo Relay (1.0)
hvap	124.27	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	0.42		Cheméo Relay (1.0)
logp	0.195		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
tb	591.86	K	Cheméo Relay (1.0)
tf	488.02	K	Cheméo Relay (1.0)

Sources

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=C33795185&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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