

Water-d

Other names:	Water-D1 HDO
Inchi:	InChI=1S/H2O/h1H2/i/hD
InchiKey:	XLYOFNOQVPJJNP-DYCDLGHISA-N
Formula:	DHO
SMILES:	O
Mol. weight [g/mol]:	19.02
CAS:	14940-63-7

Physical Properties

Property code	Value	Unit	Source
ie	12.63	eV	NIST Webbook
log10ws	0.73		Crippen Method
logp	-0.825		Crippen Method
mcvol	16.730	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14940637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/35-345-0/Water-d.pdf>

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