

Water-t

Inchi: InChI=1S/H2O/h1H2/i/hT
InchiKey: XLYOFNOQVPJJNP-MNYXATJNSA-N
Formula: HOT
SMILES: O
Mol. weight [g/mol]: 20.02
CAS: 13670-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.73		Crippen Method
logp	-0.825		Crippen Method
mcvol	16.730	ml/mol	McGowan Method
pc	21410.00 ± 300.00	kPa	NIST Webbook
rhoc	392.46 ± 10.01	kg/m ³	NIST Webbook
tc	641.70 ± 2.00	K	NIST Webbook

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=C13670172&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rhoc: Critical density
tc: Critical Temperature

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<https://www.chemeo.com/cid/28-265-7/Water-t.pdf>

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