

Deuterium oxide

Other names:	HEAVY WATER
Inchi:	InChI=1S/H2O/h1H2/i/hD2
InchiKey:	XLYOFNOQVPJJNP-ZSJDYOACSA-N
Formula:	D2O
SMILES:	[2H]O[2H]
Mol. weight [g/mol]:	20.03
CAS:	7789-20-0

Physical Properties

Property code	Value	Unit	Source
logp	-0.825		Crippen Method
mcvol	16.730	ml/mol	McGowan Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.65518e+01
Coeff. B	-3.93505e+03
Coeff. C	-4.48000e+01
Temperature range (K), min.	276.97
Temperature range (K), max.	643.89

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	9.35166e+01
Coeff. B	-8.36079e+03
Coeff. C	-1.14621e+01
Coeff. D	9.74840e-06
Temperature range (K), min.	277.15
Temperature range (K), max.	386.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1899
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010117&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1899
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure

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