deuterium oxide

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

Physical Properties

Property code	Value	Unit	Source
ie	12.64 ± 0.01	eV	NIST Webbook
ie	17.26	eV	NIST Webbook
ie	13.70	eV	NIST Webbook
ie	12.62 ± 0.01	eV	NIST Webbook
ie	12.64 ± 0.00	eV	NIST Webbook
ie	12.65 ± 0.03	eV	NIST Webbook
ie	12.64	eV	NIST Webbook
ie	12.64	eV	NIST Webbook
ie	12.64	eV	NIST Webbook
ie	12.63 ± 0.00	eV	NIST Webbook
ie	12.63 ± 0.00	eV	NIST Webbook
ie	12.64 ± 0.01	eV	NIST Webbook
ie	12.63	eV	NIST Webbook
log10ws	0.73		Crippen Method
logp	-0.825		Crippen Method
mcvol	16.730	ml/mol	McGowan Method
pc	21671.00 ± 15.00	kPa	NIST Webbook
pc	21671.00 ± 70.00	kPa	NIST Webbook
rhoc	356.49 ± 4.01	kg/m3	NIST Webbook
rhoc	356.49 ± 4.01	kg/m3	NIST Webbook
tc	643.89 ± 0.20	K	NIST Webbook
tc	643.89 ± 0.20	K	NIST Webbook
tc	0.00	K	NIST Webbook
tf	276.97 ± 0.03	K	NIST Webbook
tf	276.97 ± 0.05	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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(Pvp) = 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: https://www.chemeo.com/doc/models/crippen_log10ws

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1899

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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 Pure (Korean Thermophysical Properties Databank): https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1899

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1899

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
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
tc:	Critical Temperature
tf:	Normal melting (fusion) point