

Deuterium

Other names:	D2 UN 1957 deuterium, diatomic
Inchi:	InChI=1S/H2/h1H/i1+1D
InchiKey:	UFHFLCQGNIYNRP-VVKOMZTBSA-N
Formula:	D2
SMILES:	[H][H]
Mol. weight [g/mol]:	4.03
CAS:	7782-39-0

Physical Properties

Property code	Value	Unit	Source
gf	53.88	kJ/mol	Joback Method
hf	68.29	kJ/mol	Joback Method
hfus	-0.88	kJ/mol	Joback Method
hvap	15.30	kJ/mol	Joback Method
log10ws	0.18		Crippen Method
logp	0.246		Crippen Method
mcvol	10.860	ml/mol	McGowan Method
pc	7014.41	kPa	Joback Method
tb	198.00	K	Joback Method
tc	339.04	K	Joback Method
tf	122.50	K	Joback Method
vc	0.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	-10.08	J/molxK	198.00	Joback Method
cpg	-4.12	J/molxK	315.53	Joback Method
cpg	-4.82	J/molxK	292.03	Joback Method
cpg	-5.74	J/molxK	268.52	Joback Method
cpg	-6.92	J/molxK	245.01	Joback Method
cpg	-8.36	J/molxK	221.51	Joback Method

cpg	-3.65	J/molxK	339.04	Joback Method
dvisc	0.0000013	Paxs	198.00	Joback Method
dvisc	0.0000011	Paxs	185.42	Joback Method
dvisc	0.0000009	Paxs	172.83	Joback Method
dvisc	0.0000007	Paxs	160.25	Joback Method
dvisc	0.0000005	Paxs	147.67	Joback Method
dvisc	0.0000003	Paxs	135.08	Joback Method
dvisc	0.0000002	Paxs	122.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.25267e+01
Coeff. B	-2.12329e+02
Coeff. C	3.20000e+00
Temperature range (K), min.	18.73
Temperature range (K), max.	38.35

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.12815e+01
Coeff. B	-1.57895e+02
Coeff. C	-3.01247e-04
Coeff. D	1.05352e-07
Temperature range (K), min.	19.15
Temperature range (K), max.	25.15

Sources

Solubilities of gases in cycloethers. The solubility of 13 nonpolar gases in 2,6-dimethyltetrahydrofuran at 273.15 K and 101.32 kPa: McGowan Method:

<https://www.doi.org/10.1016/j.jct.2018.12.037>

2018-12-07

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7782390&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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1898>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mccvol: McGowan's characteristic volume
pc: Critical Pressure
pvap: Vapor pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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