

deuterium hydride

Inchi:	InChI=1S/H2/h1H/i1+1
InchiKey:	UFHFLCQGNIYNRP-OUBTZVSYSA-N
Formula:	DH
SMILES:	[H][H]
Mol. weight [g/mol]:	3.02
CAS:	13983-20-5

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
ie	15.44	eV	NIST Webbook
ie	15.44	eV	NIST Webbook
ie	15.44 ± 0.00	eV	NIST Webbook
ie	15.46	eV	NIST Webbook
log10ws	0.18		Crippen Method
logp	0.246		Crippen Method
mvol	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
tt	16.60 ± 0.20	K	NIST Webbook
vc	0.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	-10.08	J/mol×K	198.00	Joback Method
cpg	-8.36	J/mol×K	221.51	Joback Method
cpg	-6.92	J/mol×K	245.01	Joback Method
cpg	-5.74	J/mol×K	268.52	Joback Method

cpg	-4.82	J/molxK	292.03	Joback Method
cpg	-4.12	J/molxK	315.53	Joback Method
cpg	-3.65	J/molxK	339.04	Joback Method
dvisc	0.0000002	Paxs	122.50	Joback Method
dvisc	0.0000003	Paxs	135.08	Joback Method
dvisc	0.0000005	Paxs	147.67	Joback Method
dvisc	0.0000007	Paxs	160.25	Joback Method
dvisc	0.0000009	Paxs	172.83	Joback Method
dvisc	0.0000011	Paxs	185.42	Joback Method
dvisc	0.0000013	Paxs	198.00	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13983205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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