

Deuterium

Inchi:	InChI=1S/H/i1+1
InchiKey:	YZCKVEUIGOORGS-OUBTZVSYSA-N
Formula:	D
SMILES:	[H]
Mol. weight [g/mol]:	2.01
CAS:	16873-17-9

Physical Properties

Property code	Value	Unit	Source
ea	0.75 ± 0.00	eV	NIST Webbook
ea	0.75 ± 0.00	eV	NIST Webbook
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	13.60	eV	NIST Webbook
ie	13.60	eV	NIST Webbook
log10ws	0.68		Crippen Method
logp	0.113		Crippen Method
mcvol	8.710	ml/mol	McGowan Method
pc	7406.07	kPa	Joback Method
tb	198.00	K	Joback Method
tc	339.04	K	Joback Method
tf	122.50	K	Joback Method
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/mol×K	292.03	Joback Method

cpg	-4.12	J/mol×K	315.53	Joback Method
cpg	-3.65	J/mol×K	339.04	Joback Method
dvisc	0.0000001	Paxs	122.50	Joback Method
dvisc	0.0000002	Paxs	135.08	Joback Method
dvisc	0.0000002	Paxs	147.67	Joback Method
dvisc	0.0000003	Paxs	160.25	Joback Method
dvisc	0.0000004	Paxs	172.83	Joback Method
dvisc	0.0000005	Paxs	185.42	Joback Method
dvisc	0.0000007	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=C16873179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
vc:	Critical Volume

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