

Methyl-d3 radical

Inchi:	InChI=1S/CH3/h1H3/i1D3
InchiKey:	WCYWZMWISLQXQU-FIBGUPNXSA-N
Formula:	CD3
SMILES:	[CH3]
Mol. weight [g/mol]:	18.05
CAS:	2122-44-3

Physical Properties

Property code	Value	Unit	Source
gf	9.92	kJ/mol	Joback Method
hf	-8.16	kJ/mol	Joback Method
hfus	0.03	kJ/mol	Joback Method
hvap	17.67	kJ/mol	Joback Method
ie	9.83 ± 0.00	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.83 ± 0.01	eV	NIST Webbook
log10ws	0.15		Crippen Method
logp	0.450		Crippen Method
mcvol	22.800	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
tb	221.58	K	Joback Method
tc	370.90	K	Joback Method
tf	117.40	K	Joback Method
vc	0.083	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	15.82	J/mol×K	221.58	Joback Method
cpg	27.47	J/mol×K	346.02	Joback Method
cpg	25.49	J/mol×K	321.13	Joback Method
cpg	23.34	J/mol×K	296.24	Joback Method
cpg	21.02	J/mol×K	271.35	Joback Method
cpg	18.52	J/mol×K	246.47	Joback Method

cpg	29.30	J/mol×K	370.90	Joback Method
dvisc	0.0000294	Paxs	221.58	Joback Method
dvisc	0.0000289	Paxs	204.22	Joback Method
dvisc	0.0000282	Paxs	186.85	Joback Method
dvisc	0.0000275	Paxs	169.49	Joback Method
dvisc	0.0000266	Paxs	152.13	Joback Method
dvisc	0.0000255	Paxs	134.76	Joback Method
dvisc	0.0000241	Paxs	117.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2122443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
vc:	Critical Volume

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