Methan-d3-ol

Other names:	Methanol-d3
	CD3OH
	(2H3)methanol
Inchi:	InChI=1S/CH4O/c1-2/h2H,1H3/i1D3
InchiKey:	OKKJLVBELUTLKV-FIBGUPNXSA-N
Formula:	CHD3O
SMILES:	CO
Mol. weight [g/mol]:	35.06
CAS:	1849-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-179.28	kJ/mol	Joback Method
hf	-216.20	kJ/mol	Joback Method
hfus	2.43	kJ/mol	Joback Method
hvap	34.50	kJ/mol	Joback Method
ie	10.98	eV	NIST Webbook
ie	10.80 ± 0.10	eV	NIST Webbook
log10ws	0.50		Crippen Method
logp	-0.391		Crippen Method
mcvol	30.820	ml/mol	McGowan Method
pc	6696.65	kPa	Joback Method
tb	314.46	K	Joback Method
tc	475.49	K	Joback Method
tf	161.85	K	Joback Method
vc	0.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	43.33	J/mol×K	314.46	Joback Method
cpg	45.91	J/mol×K	341.30	Joback Method
cpg	48.42	J/mol×K	368.14	Joback Method
cpg	50.86	J/mol×K	394.98	Joback Method

cpg	53.23	J/mol×K	421.82	Joback Method
cpg	55.53	J/mol×K	448.65	Joback Method
cpg	57.76	J/mol×K	475.49	Joback Method
cpl	84.80	J/mol×K	298.15	NIST Webbook
dvisc	0.2499445	Pa×s	161.85	Joback Method
dvisc	0.0420484	Pa×s	187.28	Joback Method
dvisc	0.0108336	Pa×s	212.72	Joback Method
dvisc	0.0037291	Pa×s	238.15	Joback Method
dvisc	0.0015769	Pa×s	263.59	Joback Method
dvisc	0.0007759	Pa×s	289.02	Joback Method
dvisc	0.0004282	Pa×s	314.46	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1849292&Units=SI

Legend

cpg: Ideal gas heat capacity
cpl: Liquid phase 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