Methyl-d1 radical, oxo-

Inchi: InChI=1S/CHO/c1-2/h1H/i1D
InchiKey: CFHIDWOYWUOIHU-MICDWDOJSA-N
Formula: CDO
SMILES: [CH]=O
Mol. weight [g/mol]: 30.02
CAS: 24286-05-3

Physical Properties

Property code	Value	Unit	Source
ea	0.30 ± 0.01	eV	NIST Webbook
gf	-89.60	kJ/mol	Joback Method
hf	-93.74	kJ/mol	Joback Method
hfus	2.32	kJ/mol	Joback Method
hvap	24.39	kJ/mol	Joback Method
ie	8.56 ± 0.01	eV	NIST Webbook
log10ws	-4.11		Crippen Method
logp	-0.274		Crippen Method
mcvol	24.370	ml/mol	McGowan Method
pc	6990.97	kPa	Joback Method
tb	270.24	K	Joback Method
tc	436.48	K	Joback Method
tf	159.40	K	Joback Method
vc	0.100	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	25.89	J/mol×K	270.24	Joback Method
cpg	33.80	J/mol×K	408.77	Joback Method
cpg	32.58	J/mol×K	381.07	Joback Method
cpg	31.19	J/mol×K	353.36	Joback Method
cpg	29.62	J/mol×K	325.65	Joback Method
cpg	27.86	J/mol×K	297.95	Joback Method
cpg	34.87	J/mol×K	436.48	Joback Method

dvisc	0.0001213	Pa×s	270.24	Joback Method
dvisc	0.0001261	Pa×s	251.77	Joback Method
dvisc	0.0001319	Pa×s	233.29	Joback Method
dvisc	0.0001390	Pa×s	214.82	Joback Method
dvisc	0.0001480	Pa×s	196.35	Joback Method
dvisc	0.0001596	Pa×s	177.87	Joback Method
dvisc	0.0001752	Pa×s	159.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24286053&Units=SI
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

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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