

Peroxide, dimethyl

Other names:	Methyl peroxide Dimethyl peroxide (CH3O)2
Inchi:	InChI=1S/C2H6O2/c1-3-4-2/h1-2H3
InchiKey:	SRXOCFMDUSFFAK-UHFFFAOYSA-N
Formula:	C2H6O2
SMILES:	COOC
Mol. weight [g/mol]:	62.07
CAS:	690-02-8

Physical Properties

Property code	Value	Unit	Source
affp	674.00	kJ/mol	NIST Webbook
chg	-1519.00 ± 1.00	kJ/mol	NIST Webbook
gf	-244.04	kJ/mol	Joback Method
hf	-126.00	kJ/mol	NIST Webbook
hfus	3.31	kJ/mol	Joback Method
hvap	24.87	kJ/mol	Joback Method
ie	9.71	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	0.18		Crippen Method
logp	0.194		Crippen Method
mcvol	50.780	ml/mol	McGowan Method
pc	4795.85	kPa	Joback Method
tb	290.00	K	Joback Method
tc	453.25	K	Joback Method
tf	156.76	K	Joback Method
vc	0.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	80.78	J/mol×K	290.00	Joback Method
cpg	84.15	J/mol×K	317.21	Joback Method

cpg	87.59	J/mol×K	344.42	Joback Method
cpg	91.07	J/mol×K	371.63	Joback Method
cpg	94.61	J/mol×K	398.84	Joback Method
cpg	98.17	J/mol×K	426.05	Joback Method
cpg	101.75	J/mol×K	453.25	Joback Method
dvisc	0.0014381	Pa×s	156.76	Joback Method
dvisc	0.0007987	Pa×s	178.97	Joback Method
dvisc	0.0005051	Pa×s	201.17	Joback Method
dvisc	0.0003499	Pa×s	223.38	Joback Method
dvisc	0.0002590	Pa×s	245.59	Joback Method
dvisc	0.0002016	Pa×s	267.79	Joback Method
dvisc	0.0001630	Pa×s	290.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C690028&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

affp:	Proton affinity
chg:	Standard gas enthalpy of combustion
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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