

Methyl glyoxal

Other names:	Pyruvaldehyde
	Propanal, 2-oxo-
	«alpha»-Ketopropionaldehyde
	Acetylformaldehyde
	Acetylformyl
	Pyroracemic aldehyde
	Pyruvic aldehyde
	2-Ketopropionaldehyde
	2-Oxopropanal
	1,2-Propanedione
	CH3COCHO
	Glyoxal, methyl
	Propanedione
	Propanolone
	Propionaldehyde, 2-keto
	Propionaldehyde, 2-oxo-
	1-Ketopropionaldehyde
	NSC 79019
	2-Oxopropionaldehyde
	NSC 626580
Inchi:	InChI=1S/C3H4O2/c1-3(5)2-4/h2H,1H3
InchiKey:	AIJULSRZWUXGPQ-UHFFFAOYSA-N
Formula:	C3H4O2
SMILES:	CC(=O)C=O
Mol. weight [g/mol]:	72.06
CAS:	78-98-8

Physical Properties

Property code	Value	Unit	Source
chl	-1443.00 ± 4.20	kJ/mol	NIST Webbook
chl	-1446.00	kJ/mol	NIST Webbook
gf	-254.06	kJ/mol	Joback Method
hf	-271.00 ± 5.00	kJ/mol	NIST Webbook
hfl	-309.00 ± 4.20	kJ/mol	NIST Webbook
hfus	7.41	kJ/mol	Joback Method
hvap	38.00	kJ/mol	NIST Webbook
hvap	38.00 ± 2.00	kJ/mol	NIST Webbook

ie	10.00	eV	NIST Webbook
ie	9.60 ± 0.06	eV	NIST Webbook
log10ws	0.36		Crippen Method
logp	-0.226		Crippen Method
mcvol	56.270	ml/mol	McGowan Method
pc	5335.72	kPa	Joback Method
ripol	970.00		NIST Webbook
ripol	970.00		NIST Webbook
tb	345.20	K	NIST Webbook
tc	559.14	K	Joback Method
tf	215.50	K	Joback Method
vc	0.227	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.19	J/mol×K	370.57	Joback Method
cpg	113.40	J/mol×K	527.71	Joback Method
cpg	109.33	J/mol×K	496.28	Joback Method
cpg	105.08	J/mol×K	464.85	Joback Method
cpg	100.64	J/mol×K	433.43	Joback Method
cpg	96.01	J/mol×K	402.00	Joback Method
cpg	117.29	J/mol×K	559.14	Joback Method
dvisc	0.0003626	Pa×s	370.57	Joback Method
dvisc	0.0004467	Pa×s	344.73	Joback Method
dvisc	0.0005694	Pa×s	318.88	Joback Method
dvisc	0.0007574	Pa×s	293.03	Joback Method
dvisc	0.0010648	Pa×s	267.19	Joback Method
dvisc	0.0016100	Pa×s	241.34	Joback Method
dvisc	0.0026884	Pa×s	215.50	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=C78988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid 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
hfl:	Liquid phase 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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