Acetic acid, oxo-, methyl ester

Other names:	Methyl glyoxylate
	Glyoxylic acid methyl ester
	Methyl oxoethanoate
	methyl oxoacetate
Inchi:	InChI=1S/C3H4O3/c1-6-3(5)2-4/h2H,1H3
InchiKey:	KFKXSMSQHIOMSO-UHFFFAOYSA-N
Formula:	C3H4O3
SMILES:	COC(=O)C=O
Mol. weight [g/mol]:	88.06
CAS:	922-68-9

Physical Properties

Property code	Value	Unit	Source
gf	-359.06	kJ/mol	Joback Method
hf	-435.63	kJ/mol	Joback Method
hfpi	937.00 ± 4.00	kJ/mol	NIST Webbook
hfus	8.60	kJ/mol	Joback Method
hvap	38.15	kJ/mol	Joback Method
log10ws	0.78		Crippen Method
logp	-0.642		Crippen Method
mcvol	62.140	ml/mol	McGowan Method
pc	5205.63	kPa	Joback Method
tb	392.99	K	Joback Method
tc	581.64	K	Joback Method
tf	237.73	K	Joback Method
vc	0.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	109.13	J/mol×K	392.99	Joback Method
cpg	131.40	J/mol×K	550.20	Joback Method
cpg	127.20	J/mol×K	518.76	Joback Method
cpg	122.86	J/mol×K	487.32	Joback Method

cpg	118.40	J/mol×K	455.87	Joback Method
cpg	113.82	J/mol×K	424.43	Joback Method
cpg	135.46	J/mol×K	581.64	Joback Method
dvisc	0.0003506	Pa×s	392.99	Joback Method
dvisc	0.0004312	Pa×s	367.11	Joback Method
dvisc	0.0005472	Pa×s	341.24	Joback Method
dvisc	0.0007222	Pa×s	315.36	Joback Method
dvisc	0.0010016	Pa×s	289.48	Joback Method
dvisc	0.0014812	Pa×s	263.61	Joback Method
dvisc	0.0023853	Pa×s	237.73	Joback Method

Sources

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=C922689&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfpi: Enthalpy of formation of positive ion at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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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