

Acetic acid, methoxy-, methyl ester

Other names:	CBC 108569 Methoxyacetic acid methyl ester Methoxymethyl acetate methoxyacetic acid, methyl ester methyl .alpha.-methoxyacetate methyl 2-methoxyacetate methyl methoxyacetate
Inchi:	InChI=1S/C4H8O3/c1-6-3-4(5)7-2/h3H2,1-2H3
InchiKey:	QRMHDGWGLNLHMN-UHFFFAOYSA-N
Formula:	C4H8O3
SMILES:	COCC(=O)OC
Mol. weight [g/mol]:	104.10
CAS:	6290-49-9

Physical Properties

Property code	Value	Unit	Source
gf	-356.12	kJ/mol	Joback Method
hf	-502.91	kJ/mol	Joback Method
hfus	10.09	kJ/mol	Joback Method
hvap	47.20 ± 4.20	kJ/mol	NIST Webbook
ie	9.56 ± 0.05	eV	NIST Webbook
log10ws	0.55		Crippen Method
logp	-0.194		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	402.70	K	NIST Webbook
tb	404.20	K	NIST Webbook
tc	569.26	K	Joback Method
tf	229.23	K	Joback Method
vc	0.301	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	149.26	J/molxK	389.63	Joback Method
cpg	156.06	J/molxK	419.57	Joback Method
cpg	162.75	J/molxK	449.51	Joback Method
cpg	169.33	J/molxK	479.44	Joback Method
cpg	175.78	J/molxK	509.38	Joback Method
cpg	182.09	J/molxK	539.32	Joback Method
cpg	188.25	J/molxK	569.26	Joback Method
dvisc	0.0020724	Paxs	229.23	Joback Method
dvisc	0.0012119	Paxs	255.96	Joback Method
dvisc	0.0007844	Paxs	282.70	Joback Method
dvisc	0.0005474	Paxs	309.43	Joback Method
dvisc	0.0004044	Paxs	336.16	Joback Method
dvisc	0.0003125	Paxs	362.90	Joback Method
dvisc	0.0002501	Paxs	389.63	Joback Method
hvapt	39.30	kJ/mol	297.50	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6290499&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Phase Behavior for the CO₂ + Methyl Methoxyacetate and CO₂ + Methyl Methacrylate Systems at Pressures from (5 to 20) MPa and Various Temperatures:

<https://www.doi.org/10.1021/acs.jced.5b00711>

https://en.wikipedia.org/wiki/Joback_method

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mconvol:	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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