

Acetic acid, methoxy-

Other names:	2-Methoxyacetic acid CH ₃ OCH ₂ COOH Methoxyacetic acid Methoxyethanoic acid
Inchi:	InChI=1S/C3H6O3/c1-6-2-3(4)5/h2H2,1H3,(H,4,5)
InchiKey:	RMIODHQZRUFFFF-UHFFFAOYSA-N
Formula:	C ₃ H ₆ O ₃
SMILES:	COCC(=O)O
Mol. weight [g/mol]:	90.08
CAS:	625-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-396.36	kJ/mol	Joback Method
hf	-502.28	kJ/mol	Joback Method
hfus	10.40	kJ/mol	Joback Method
hvap	48.11	kJ/mol	Joback Method
log10ws	0.74		Crippen Method
logp	-0.283		Crippen Method
mcvol	66.440	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
tb	476.70	K	NIST Webbook
tc	611.34	K	Joback Method
tf	256.55	K	Joback Method
vc	0.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.17	J/mol×K	611.34	Joback Method
cpg	129.32	J/mol×K	436.51	Joback Method
cpg	134.49	J/mol×K	465.65	Joback Method
cpg	139.52	J/mol×K	494.79	Joback Method
cpg	144.41	J/mol×K	523.92	Joback Method

cpg	149.15	J/molxK	553.06	Joback Method
cpg	153.74	J/molxK	582.20	Joback Method
dvisc	0.0002559	Paxs	436.51	Joback Method
dvisc	0.0190072	Paxs	256.55	Joback Method
dvisc	0.0063665	Paxs	286.54	Joback Method
dvisc	0.0026236	Paxs	316.54	Joback Method
dvisc	0.0012605	Paxs	346.53	Joback Method
dvisc	0.0006806	Paxs	376.52	Joback Method
dvisc	0.0004025	Paxs	406.52	Joback Method
hvapt	54.50	kJ/mol	401.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57677e+01
Coeff. B	-4.30386e+03
Coeff. C	-9.06830e+01
Temperature range (K), min.	368.71
Temperature range (K), max.	504.35

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=C625456&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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