

Methanol, chloro-, acetate

Other names:	Chloromethyl ethanoate Chloromethyl acetate
Inchi:	InChI=1S/C3H5ClO2/c1-3(5)6-2-4/h2H2,1H3
InchiKey:	SMJYMSAPPGLBAR-UHFFFAOYSA-N
Formula:	C3H5ClO2
SMILES:	CC(=O)OCCI
Mol. weight [g/mol]:	108.52
CAS:	625-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-271.47	kJ/mol	Joback Method
hf	-365.79	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	35.81	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.746		Crippen Method
mvol	72.810	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
rinpol	680.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	680.00		NIST Webbook
ripol	1181.00		NIST Webbook
ripol	1174.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1164.00		NIST Webbook
tb	381.76	K	Joback Method
tc	570.48	K	Joback Method
tf	225.65	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.88	J/molxK	381.76	Joback Method
cpg	123.10	J/molxK	413.21	Joback Method
cpg	128.19	J/molxK	444.67	Joback Method
cpg	133.14	J/molxK	476.12	Joback Method
cpg	137.95	J/molxK	507.57	Joback Method
cpg	142.60	J/molxK	539.02	Joback Method
cpg	147.10	J/molxK	570.48	Joback Method
dvisc	0.0025693	Paxs	225.65	Joback Method
dvisc	0.0015292	Paxs	251.67	Joback Method
dvisc	0.0010031	Paxs	277.69	Joback Method
dvisc	0.0007073	Paxs	303.70	Joback Method
dvisc	0.0005270	Paxs	329.72	Joback Method
dvisc	0.0004099	Paxs	355.74	Joback Method
dvisc	0.0003300	Paxs	381.76	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=C625569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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