

Methyl iodoacetate

Inchi:	InChI=1S/C3H5IO2/c1-6-3(5)2-4/h2H2,1H3
InchiKey:	YDGMIJCIBXSCQR-UHFFFAOYSA-N
Formula:	C3H5IO2
SMILES:	COC(=O)CI
Mol. weight [g/mol]:	199.98

Physical Properties

Property code	Value	Unit	Source
gf	-201.42	kJ/mol	Joback Method
hf	-273.18	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	40.80	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.594		Crippen Method
mcvol	86.390	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
rinpol	886.00		NIST Webbook
tb	437.47	K	Joback Method
tc	656.53	K	Joback Method
tf	253.79	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.84	J/molxK	437.47	Joback Method
cpg	156.53	J/molxK	620.02	Joback Method
cpg	151.87	J/molxK	583.51	Joback Method
cpg	146.98	J/molxK	547.00	Joback Method
cpg	141.84	J/molxK	510.49	Joback Method
cpg	136.46	J/molxK	473.98	Joback Method
cpg	160.95	J/molxK	656.53	Joback Method
dvisc	0.0004213	Paxs	437.47	Joback Method
dvisc	0.0005284	Paxs	406.86	Joback Method

dvisc	0.0006875	Paxs	376.24	Joback Method
dvisc	0.0009373	Paxs	345.63	Joback Method
dvisc	0.0013573	Paxs	315.02	Joback Method
dvisc	0.0021284	Paxs	284.40	Joback Method
dvisc	0.0037202	Paxs	253.79	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=R248367&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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