

2-Propenoic acid, 3-iodo, methyl ester, (Z)-

Inchi:	InChI=1S/C4H5IO2/c1-7-4(6)2-3-5/h2-3H,1H3/b3-2-
InchiKey:	SUQXOFVGKSUSSM-IHWYPQMZSA-N
Formula:	C4H5IO2
SMILES:	COC(=O)C=CI
Mol. weight [g/mol]:	211.99
CAS:	6214-23-9

Physical Properties

Property code	Value	Unit	Source
gf	-112.78	kJ/mol	Joback Method
hf	-176.60	kJ/mol	Joback Method
hfus	13.51	kJ/mol	Joback Method
hvap	42.98	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.108		Crippen Method
mcvol	96.180	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	464.51	K	Joback Method
tc	691.60	K	Joback Method
tf	259.98	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.47	J/molxK	464.51	Joback Method
cpg	178.22	J/molxK	653.75	Joback Method
cpg	173.19	J/molxK	615.90	Joback Method
cpg	167.82	J/molxK	578.06	Joback Method
cpg	162.09	J/molxK	540.21	Joback Method
cpg	155.98	J/molxK	502.36	Joback Method
cpg	182.93	J/molxK	691.60	Joback Method
dvisc	0.0003280	Paxs	464.51	Joback Method
dvisc	0.0004155	Paxs	430.42	Joback Method

dvisc	0.0005482	Paxs	396.33	Joback Method
dvisc	0.0007620	Paxs	362.25	Joback Method
dvisc	0.0011343	Paxs	328.16	Joback Method
dvisc	0.0018514	Paxs	294.07	Joback Method
dvisc	0.0034362	Paxs	259.98	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=C6214239&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
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
mccvol:	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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