acetic acid, 2-iodo-, 1-methylethyl ester

Other names: propan-2-yl iodoacetate
Isopropyl iodoacetate
Inchi: InChI=1S/C5H9IO2/c1-4(2)8-5(7)3-6/h4H,3H2,1-2H3
InchiKey: AGQAITFOQLGIGK-UHFFFAOYSA-N
Formula: C5H9IO2
SMILES: CC(C)OC(=O)CI
Mol. weight [g/mol]: 228.03

Physical Properties

Property code	Value	Unit	Source
gf	-187.02	kJ/mol	Joback Method
hf	-319.74	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.373		Crippen Method
mcvol	114.570	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	999.90		NIST Webbook
tb	482.79	K	Joback Method
tc	700.64	K	Joback Method
tf	261.33	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.38	J/mol×K	482.79	Joback Method
cpg	214.35	J/mol×K	519.10	Joback Method
cpg	222.88	J/mol×K	555.41	Joback Method
cpg	230.98	J/mol×K	591.71	Joback Method
cpg	238.66	J/mol×K	628.02	Joback Method
cpg	245.92	J/mol×K	664.33	Joback Method
cpg	252.77	J/mol×K	700.64	Joback Method

dvisc	0.0050974	Pa×s	261.33	Joback Method
dvisc	0.0024550	Pa×s	298.24	Joback Method
dvisc	0.0013888	Pa×s	335.15	Joback Method
dvisc	0.0008796	Pa×s	372.06	Joback Method
dvisc	0.0006050	Pa×s	408.97	Joback Method
dvisc	0.0004428	Pa×s	445.88	Joback Method
dvisc	0.0003398	Pa×s	482.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U400955&Units=SI

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