Isobutyl iodoacetate

Inchi: InChI=1S/C6H11IO2/c1-5(2)4-9-6(8)3-7/h5H,3-4H2,1-2H3
InchiKey: HFVPSCYRMKGRBZ-UHFFFAOYSA-N
Formula: C6H11IO2
SMILES: CC(C)COC(=O)CI
Mol. weight [g/mol]: 242.05

Physical Properties

Property code	Value	Unit	Source
gf	-178.60	kJ/mol	Joback Method
hf	-340.38	kJ/mol	Joback Method
hfus	14.97	kJ/mol	Joback Method
hvap	47.09	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.621		Crippen Method
mcvol	128.660	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	505.67	K	Joback Method
tc	720.10	K	Joback Method
tf	272.60	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.84	J/mol×K	505.67	Joback Method
cpg	292.19	J/mol×K	684.36	Joback Method
cpg	283.90	J/mol×K	648.62	Joback Method
cpg	275.13	J/mol×K	612.88	Joback Method
cpg	265.87	J/mol×K	577.15	Joback Method
cpg	256.11	J/mol×K	541.41	Joback Method
cpg	300.01	J/mol×K	720.10	Joback Method
dvisc	0.0003082	Pa×s	505.67	Joback Method
dvisc	0.0004035	Pa×s	466.83	Joback Method
dvisc	0.0005547	Pa×s	427.98	Joback Method

dvisc	0.0008126	Pa×s	389.13	Joback Method
dvisc	0.0012956	Pa×s	350.29	Joback Method
dvisc	0.0023206	Pa×s	311.45	Joback Method
dvisc	0.0049075	Pa×s	272.60	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=R248332&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume