Isobutyl chloroformate

Other names:	Carbonochloridic acid, 2-methylpropyl ester
	Chlorocarbonic acid isobutyl ester
	Chloroformic acid isobutyl ester
	Formic acid, chloro-, isobutyl ester
	Isobutyl chlorocarbonate
	2-Methylpropyl carbonochloridate
	2-Methylpropyl chloroformate
	Isobutyl chloridocarbonate
	NSC 8429
Inchi:	InChI=1S/C5H9ClO2/c1-4(2)3-8-5(6)7/h4H,3H2,1-2H3
InchiKey:	YOETUEMZNOLGDB-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	CC(C)COC(=O)Cl
Mol. weight [g/mol]:	136.58
CAS:	543-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-257.07	kJ/mol	Joback Method
hf	-412.35	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	39.88	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	2.018		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	808.00		NIST Webbook
tb	402.00	K	NIST Webbook
tc	617.43	K	Joback Method
tf	233.19	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.92	J/mol×K	427.08	Joback Method
cpg	195.50	J/mol×K	458.81	Joback Method
cpg	203.77	J/mol×K	490.53	Joback Method
cpg	211.73	J/mol×K	522.26	Joback Method
cpg	219.39	J/mol×K	553.98	Joback Method
cpg	226.73	J/mol×K	585.71	Joback Method
cpg	233.77	J/mol×K	617.43	Joback Method
dvisc	0.0042591	Pa×s	233.19	Joback Method
dvisc	0.0020958	Pa×s	265.50	Joback Method
dvisc	0.0012028	Pa×s	297.82	Joback Method
dvisc	0.0007696	Pa×s	330.13	Joback Method
dvisc	0.0005332	Pa×s	362.45	Joback Method
dvisc	0.0003923	Pa×s	394.76	Joback Method
dvisc	0.0003024	Pa×s	427.08	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C543271&Units=SI
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

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