Propionic acid, 2,3-dichloro-2-chloromethyl-, methyl ester

Inchi: InChI=1S/C5H7Cl3O2/c1-10-4(9)5(8,2-6)3-7/h2-3H2,1H3
InchiKey: KLXRARKCCAQPMU-UHFFFAOYSA-N
Formula: C5H7Cl3O2
SMILES: COC(=O)C(Cl)(CCl)CCl
Mol. weight [g/mol]: 205.47
CAS: 116594-64-0

Physical Properties

Property code	Value	Unit	Source
gf	-275.65	kJ/mol	Joback Method
hf	-447.30	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	47.74	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.615		Crippen Method
mcvol	125.470	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	499.15	K	Joback Method
tc	710.20	K	Joback Method
tf	310.45	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.65	J/mol×K	499.15	Joback Method
cpg	243.00	J/mol×K	534.32	Joback Method
cpg	250.81	J/mol×K	569.50	Joback Method
cpg	258.10	J/mol×K	604.67	Joback Method
cpg	264.90	J/mol×K	639.85	Joback Method
cpg	271.22	J/mol×K	675.02	Joback Method
cpg	277.09	J/mol×K	710.20	Joback Method
dvisc	0.0032418	Pa×s	310.45	Joback Method
dvisc	0.0018441	Pa×s	341.90	Joback Method

dvisc	0.0011536	Pa×s	373.35	Joback Method
dvisc	0.0007762	Pa×s	404.80	Joback Method
dvisc	0.0005530	Pa×s	436.25	Joback Method
dvisc	0.0004123	Pa×s	467.70	Joback Method
dvisc	0.0003190	Pa×s	499.15	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=C116594640&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