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

Inchi: InChI=1S/C5H8Cl2O2/c1-5(7,3-6)4(8)9-2/h3H2,1-2H3
InchiKey: UMKUDPXEXDNELA-UHFFFAOYSA-N
Formula: C5H8Cl2O2
SMILES: COC(=O)C(C)(Cl)CCl
Mol. weight [g/mol]: 171.02
CAS: 918-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-263.72	kJ/mol	Joback Method
hf	-431.56	kJ/mol	Joback Method
hfus	12.47	kJ/mol	Joback Method
hvap	43.35	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.396		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	461.72	K	Joback Method
tc	666.97	K	Joback Method
tf	280.53	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.59	J/mol×K	461.72	Joback Method
cpg	221.52	J/mol×K	495.93	Joback Method
cpg	229.94	J/mol×K	530.14	Joback Method
cpg	237.86	J/mol×K	564.34	Joback Method
cpg	245.30	J/mol×K	598.55	Joback Method
cpg	252.27	J/mol×K	632.76	Joback Method
cpg	258.80	J/mol×K	666.97	Joback Method
dvisc	0.0037813	Pa×s	280.53	Joback Method
dvisc	0.0020747	Pa×s	310.73	Joback Method

dvisc	0.0012660	Pa×s	340.93	Joback Method
dvisc	0.0008372	Pa×s	371.12	Joback Method
dvisc	0.0005892	Pa×s	401.32	Joback Method
dvisc	0.0004356	Pa×s	431.52	Joback Method
dvisc	0.0003350	Pa×s	461.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C918785&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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