Propionic acid, 2,2-dichloro-, pentyl ester

Other names: Propanoic acid, 2,2-dichloro-, pentyl ester
Inchi: InChI=1S/C8H14Cl2O2/c1-3-4-5-6-12-7(11)8(2,9)10/h3-6H2,1-2H3
InchiKey: ZCPOSLAFHCNHBE-UHFFFAOYSA-N
Formula: C8H14Cl2O2
SMILES: CCCCCOC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]: 213.10
CAS: 17640-08-3

Physical Properties

Property code	Value	Unit	Source
gf	-238.46	kJ/mol	Joback Method
hf	-493.48	kJ/mol	Joback Method
hfus	20.24	kJ/mol	Joback Method
hvap	50.03	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.914		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
tb	530.36	K	Joback Method
tc	727.45	K	Joback Method
tf	314.34	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.84	J/mol×K	530.36	Joback Method
cpg	350.00	J/mol×K	563.21	Joback Method
cpg	361.50	J/mol×K	596.06	Joback Method
cpg	372.35	J/mol×K	628.90	Joback Method
cpg	382.59	J/mol×K	661.75	Joback Method
cpg	392.23	J/mol×K	694.60	Joback Method
cpg	401.29	J/mol×K	727.45	Joback Method
dvisc	0.0032784	Pa×s	314.34	Joback Method

dvisc	0.0016965	Pa×s	350.34	Joback Method
dvisc	0.0009926	Pa×s	386.35	Joback Method
dvisc	0.0006363	Pa×s	422.35	Joback Method
dvisc	0.0004374	Pa×s	458.35	Joback Method
dvisc	0.0003176	Pa×s	494.36	Joback Method
dvisc	0.0002408	Pa×s	530.36	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=C17640083&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