1,3-Dichloroisopropyl isopentanoate

Inchi: InChI=1S/C8H14Cl2O2/c1-6(2)4-7(11)12-8(3,10)5-9/h6H,4-5H2,1-3H3
InchiKey: HOYDHGBXJGTXGW-UHFFFAOYSA-N
Formula: C8H14Cl2O2
SMILES: CC(C)CC(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]: 213.10

Physical Properties

Property code	Value	Unit	Source
gf	-240.90	kJ/mol	Joback Method
hf	-498.76	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	49.64	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.769		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	529.92	K	Joback Method
tc	731.23	K	Joback Method
tf	299.34	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.15	J/mol×K	529.92	Joback Method
cpg	393.82	J/mol×K	697.68	Joback Method
cpg	383.99	J/mol×K	664.13	Joback Method
cpg	373.54	J/mol×K	630.58	Joback Method
cpg	362.43	J/mol×K	597.02	Joback Method
cpg	350.64	J/mol×K	563.47	Joback Method
cpg	403.04	J/mol×K	731.23	Joback Method
dvisc	0.0002269	Pa×s	529.92	Joback Method

dvisc	0.0003072	Pa×s	491.49	Joback Method
dvisc	0.0004378	Pa×s	453.06	Joback Method
dvisc	0.0006663	Pa×s	414.63	Joback Method
dvisc	0.0011049	Pa×s	376.20	Joback Method
dvisc	0.0020557	Pa×s	337.77	Joback Method
dvisc	0.0044860	Pa×s	299.34	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=R150260&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume