

1,3-Dichloroisopropyl isohecanoate

Inchi:	InChI=1S/C9H16Cl2O2/c1-7(2)4-5-8(12)13-9(3,11)6-10/h7H,4-6H2,1-3H3
InchiKey:	AQIXRRIYUDNUTN-UHFFFAOYSA-N
Formula:	C9H16Cl2O2
SMILES:	CC(C)CCC(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]:	227.13

Physical Properties

Property code	Value	Unit	Source
gf	-232.48	kJ/mol	Joback Method
hf	-519.40	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	51.87	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.160		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinsol	1356.00		NIST Webbook
tb	552.80	K	Joback Method
tc	751.28	K	Joback Method
tf	310.61	K	Joback Method
vc	0.644	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.74	J/molxK	552.80	Joback Method
cpg	397.06	J/molxK	585.88	Joback Method
cpg	409.64	J/molxK	618.96	Joback Method
cpg	421.51	J/molxK	652.04	Joback Method
cpg	432.68	J/molxK	685.12	Joback Method
cpg	443.20	J/molxK	718.20	Joback Method
cpg	453.08	J/molxK	751.28	Joback Method
dvisc	0.0041371	Paxs	310.61	Joback Method
dvisc	0.0018682	Paxs	350.98	Joback Method

dvisc	0.0009940	Paxs	391.34	Joback Method
dvisc	0.0005951	Paxs	431.70	Joback Method
dvisc	0.0003889	Paxs	472.07	Joback Method
dvisc	0.0002718	Paxs	512.43	Joback Method
dvisc	0.0002002	Paxs	552.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R150255&Units=SI

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

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