

1,3-Dichloroisopropyl pentanoate

Inchi:	InChI=1S/C8H14Cl2O2/c1-3-4-5-7(11)12-8(2,10)6-9/h3-6H2,1-2H3
InchiKey:	OEMJJSRUWZBVRG-UHFFFAOYSA-N
Formula:	C8H14Cl2O2
SMILES:	CCCCC(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]:	213.10

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
rinsol	1297.00		NIST Webbook
tb	530.36	K	Joback Method
tc	727.45	K	Joback Method
tf	314.34	K	Joback Method
vc	0.595	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.84	J/molxK	530.36	Joback Method
cpg	350.00	J/molxK	563.21	Joback Method
cpg	361.50	J/molxK	596.06	Joback Method
cpg	372.35	J/molxK	628.90	Joback Method
cpg	382.59	J/molxK	661.75	Joback Method
cpg	392.23	J/molxK	694.60	Joback Method
cpg	401.29	J/molxK	727.45	Joback Method
dvisc	0.0032784	Paxs	314.34	Joback Method
dvisc	0.0016965	Paxs	350.34	Joback Method

dvisc	0.0009926	Paxs	386.35	Joback Method
dvisc	0.0006363	Paxs	422.35	Joback Method
dvisc	0.0004374	Paxs	458.35	Joback Method
dvisc	0.0003176	Paxs	494.36	Joback Method
dvisc	0.0002408	Paxs	530.36	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=R150295&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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