

1,3-Dichloroisopropyl hexanoate

Inchi:	InChI=1S/C9H16Cl2O2/c1-3-4-5-6-8(12)13-9(2,11)7-10/h3-7H2,1-2H3
InchiKey:	HTCULUNCUAOAOX-UHFFFAOYSA-N
Formula:	C9H16Cl2O2
SMILES:	CCCCCC(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]:	227.13

Physical Properties

Property code	Value	Unit	Source
gf	-230.04	kJ/mol	Joback Method
hf	-514.12	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.304		Crippen Method
mvol	169.590	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1394.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	553.24	K	Joback Method
tc	747.71	K	Joback Method
tf	325.61	K	Joback Method
vc	0.650	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.39	J/molxK	553.24	Joback Method
cpg	396.39	J/molxK	585.65	Joback Method
cpg	408.67	J/molxK	618.06	Joback Method
cpg	420.28	J/molxK	650.48	Joback Method
cpg	431.24	J/molxK	682.89	Joback Method
cpg	441.57	J/molxK	715.30	Joback Method
cpg	451.30	J/molxK	747.71	Joback Method
dvisc	0.0030630	Paxs	325.61	Joback Method

dvisc	0.0015580	Paxs	363.55	Joback Method
dvisc	0.0009004	Paxs	401.49	Joback Method
dvisc	0.0005721	Paxs	439.43	Joback Method
dvisc	0.0003906	Paxs	477.36	Joback Method
dvisc	0.0002822	Paxs	515.30	Joback Method
dvisc	0.0002131	Paxs	553.24	Joback Method

Sources

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=R150186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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