1,3-Dichloroisopropyl heptanoate

Inchi: InChI=1S/C10H18Cl2O2/c1-3-4-5-6-7-9(13)14-10(2,12)8-11/h3-8H2,1-2H3
InchiKey: FPZTZMYOEFDHBQ-UHFFFAOYSA-N
Formula: C10H18Cl2O2
SMILES: CCCCCCC(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]: 241.16

Physical Properties

Property code	Value	Unit	Source
gf	-221.62	kJ/mol	Joback Method
hf	-534.76	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.694		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	576.12	K	Joback Method
tc	768.12	K	Joback Method
tf	336.88	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.68	J/mol×K	576.12	Joback Method
cpg	444.40	J/mol×K	608.12	Joback Method
cpg	457.38	J/mol×K	640.12	Joback Method
cpg	469.65	J/mol×K	672.12	Joback Method
cpg	481.24	J/mol×K	704.12	Joback Method
cpg	492.18	J/mol×K	736.12	Joback Method
cpg	502.48	J/mol×K	768.12	Joback Method
dvisc	0.0028380	Pa×s	336.88	Joback Method

dvisc	0.0014203	Pa×s	376.75	Joback Method
dvisc	0.0008115	Pa×s	416.63	Joback Method
dvisc	0.0005113	Pa×s	456.50	Joback Method
dvisc	0.0003469	Pa×s	496.37	Joback Method
dvisc	0.0002494	Pa×s	536.25	Joback Method
dvisc	0.0001877	Pa×s	576.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R150235&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