1,3-Dichloroisopropyl octanoate

Inchi: InChI=1S/C11H20Cl2O2/c1-3-4-5-6-7-8-10(14)15-11(2,13)9-12/h3-9H2,1-2H3
InchiKey: KRSMHCZRTSQGKM-UHFFFAOYSA-N
Formula: C11H20Cl2O2
SMILES: CCCCCCCC(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]: 255.18

Physical Properties

Property code	Value	Unit	Source
gf	-213.20	kJ/mol	Joback Method
hf	-555.40	kJ/mol	Joback Method
hfus	28.01	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.084		Crippen Method
mcvol	197.770	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	599.00	K	Joback Method
tc	788.73	K	Joback Method
tf	348.15	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.60	J/mol×K	599.00	Joback Method
cpg	493.95	J/mol×K	630.62	Joback Method
cpg	507.54	J/mol×K	662.24	Joback Method
cpg	520.40	J/mol×K	693.87	Joback Method
cpg	532.54	J/mol×K	725.49	Joback Method
cpg	544.01	J/mol×K	757.11	Joback Method
cpg	554.82	J/mol×K	788.73	Joback Method
dvisc	0.0026101	Pa×s	348.15	Joback Method

dvisc	0.0012864	Pa×s	389.96	Joback Method
dvisc	0.0007271	Pa×s	431.77	Joback Method
dvisc	0.0004545	Pa×s	473.57	Joback Method
dvisc	0.0003066	Pa×s	515.38	Joback Method
dvisc	0.0002195	Pa×s	557.19	Joback Method
dvisc	0.0001646	Pa×s	599.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R150280&Units=SI
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

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