1,3-Dichloroisopropyl nonanoate

Inchi: InChI=1S/C12H22Cl2O2/c1-3-4-5-6-7-8-9-11(15)16-12(2,14)10-13/h3-10H2,1-2H3
InchiKey: PQYSXGKADZLVDO-UHFFFAOYSA-N
Formula: C12H22Cl2O2
SMILES: CCCCCCCCC(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]: 269.21

Physical Properties

Property code	Value	Unit	Source
gf	-204.78	kJ/mol	Joback Method
hf	-576.04	kJ/mol	Joback Method
hfus	30.60	kJ/mol	Joback Method
hvap	58.94	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.474		Crippen Method
mcvol	211.860	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	621.88	K	Joback Method
tc	809.59	K	Joback Method
tf	359.42	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.06	J/mol×K	621.88	Joback Method
cpg	597.01	J/mol×K	778.31	Joback Method
cpg	585.08	J/mol×K	747.02	Joback Method
cpg	572.45	J/mol×K	715.74	Joback Method
cpg	559.09	J/mol×K	684.45	Joback Method
cpg	544.97	J/mol×K	653.17	Joback Method
cpg	608.27	J/mol×K	809.59	Joback Method
dvisc	0.0001438	Pa×s	621.88	Joback Method

dvisc	0.0001923	Pa×s	578.14	Joback Method
dvisc	0.0002698	Pa×s	534.39	Joback Method
dvisc	0.0004021	Pa×s	490.65	Joback Method
dvisc	0.0006480	Pa×s	446.91	Joback Method
dvisc	0.0011582	Pa×s	403.16	Joback Method
dvisc	0.0023843	Pa×s	359.42	Joback Method

Sources

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=R150275&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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