Dichloroacetic acid, nonyl ester

Other names: Nonyl dichloroacetate
Inchi: InChI=1S/C11H20Cl2O2/c1-2-3-4-5-6-7-8-9-15-11(14)10(12)13/h10H,2-9H2,1H3
InchiKey: XKMMRMJBZDCIHI-UHFFFAOYSA-N
Formula: C11H20Cl2O2
SMILES: CCCCCCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 255.18
CAS: 83004-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-218.48	kJ/mol	Joback Method
hf	-551.93	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.084		Crippen Method
mcvol	197.770	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1584.10		NIST Webbook
tb	601.79	K	Joback Method
tc	785.44	K	Joback Method
tf	330.73	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.80	J/mol×K	601.79	Joback Method
cpg	490.81	J/mol×K	632.40	Joback Method
cpg	504.16	J/mol×K	663.01	Joback Method
cpg	516.86	J/mol×K	693.62	Joback Method
cpg	528.94	J/mol×K	724.22	Joback Method
cpg	540.40	J/mol×K	754.83	Joback Method
cpg	551.25	J/mol×K	785.44	Joback Method

dvisc	0.0029863	Pa×s	330.73	Joback Method
dvisc	0.0013948	Pa×s	375.91	Joback Method
dvisc	0.0007671	Pa×s	421.08	Joback Method
dvisc	0.0004737	Pa×s	466.26	Joback Method
dvisc	0.0003185	Pa×s	511.44	Joback Method
dvisc	0.0002284	Pa×s	556.61	Joback Method
dvisc	0.0001722	Pa×s	601.79	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=C83004993&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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