Dichloroacetic acid, undec-2-enyl ester

Inchi: InChI=1S/C13H22Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-17-13(16)12(14)15/h9-10,12H,2-8,11H
InchiKey: CWGSMVDQCFKHOS-MDZDMXLPSA-N
Formula: C13H22Cl2O2
SMILES: CCCCCCCCC=CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 281.22

Physical Properties

Property code	Value	Unit	Source
gf	-121.42	kJ/mol	Joback Method
hf	-475.99	kJ/mol	Joback Method
hfus	37.29	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.640		Crippen Method
mcvol	221.650	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tb	651.71	K	Joback Method
tc	838.62	K	Joback Method
tf	348.19	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.07	J/mol×K	651.71	Joback Method
cpg	572.73	J/mol×K	682.86	Joback Method
cpg	586.65	J/mol×K	714.01	Joback Method
cpg	599.84	J/mol×K	745.16	Joback Method
cpg	612.34	J/mol×K	776.31	Joback Method
cpg	624.17	J/mol×K	807.47	Joback Method
cpg	635.36	J/mol×K	838.62	Joback Method
dvisc	0.0023683	Pa×s	348.19	Joback Method

dvisc	0.0010398	Pa×s	398.78	Joback Method
dvisc	0.0005494	Pa×s	449.36	Joback Method
dvisc	0.0003303	Pa×s	499.95	Joback Method
dvisc	0.0002181	Pa×s	550.54	Joback Method
dvisc	0.0001544	Pa×s	601.12	Joback Method
dvisc	0.0001153	Pa×s	651.71	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=U299436&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