Trichloroacetic acid, undec-2-enyl ester

Inchi: InChI=1S/C13H21Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-18-12(17)13(14,15)16/h9-10H,2-8,11H
InchiKey: HPCFGWRDJUTDBB-MDZDMXLPSA-N
Formula: C13H21Cl3O2
SMILES: CCCCCCCCC=CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 315.66

Physical Properties

Property code	Value	Unit	Source
gf	-128.07	kJ/mol	Joback Method
hf	-495.20	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.207		Crippen Method
mcvol	233.890	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	1859.00		NIST Webbook
tb	686.35	K	Joback Method
tc	882.83	K	Joback Method
tf	395.53	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.67	J/mol×K	686.35	Joback Method
cpg	602.60	J/mol×K	719.10	Joback Method
cpg	615.70	J/mol×K	751.84	Joback Method
cpg	628.03	J/mol×K	784.59	Joback Method
cpg	639.63	J/mol×K	817.34	Joback Method
cpg	650.55	J/mol×K	850.08	Joback Method
cpg	660.85	J/mol×K	882.83	Joback Method
dvisc	0.0015726	Pa×s	395.53	Joback Method
dvisc	0.0007602	Pa×s	444.00	Joback Method

dvisc	0.0004240	Pa×s	492.47	Joback Method
dvisc	0.0002626	Pa×s	540.94	Joback Method
dvisc	0.0001760	Pa×s	589.41	Joback Method
dvisc	0.0001253	Pa×s	637.88	Joback Method
dvisc	0.0000936	Pa×s	686.35	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=U299261&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

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