Trichloroacetic acid, undecyl ester

Other names: Undecyl trichloroacetate
Inchi: InChI=1S/C13H23Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-18-12(17)13(14,15)16/h2-11H2,1H3
InchiKey: ZKEYPXQCWNXAQG-UHFFFAOYSA-N
Formula: C13H23Cl3O2
SMILES: CCCCCCCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 317.68
CAS: 74339-49-4

Physical Properties

Property code	Value	Unit	Source
gf	-208.29	kJ/mol	Joback Method
hf	-612.42	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.431		Crippen Method
mcvol	238.190	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook
ripol	2263.00		NIST Webbook
ripol	2263.00		NIST Webbook
tb	682.19	K	Joback Method
tc	872.30	K	Joback Method
tf	400.61	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.33	J/mol×K	682.19	Joback Method
cpg	625.80	J/mol×K	713.87	Joback Method

cpg	639.46	J/mol×K	745.56	Joback Method
cpg	652.33	J/mol×K	777.24	Joback Method
cpg	664.47	J/mol×K	808.93	Joback Method
cpg	675.89	J/mol×K	840.61	Joback Method
cpg	686.64	J/mol×K	872.30	Joback Method
dvisc	0.0016819	Pa×s	400.61	Joback Method
dvisc	0.0008389	Pa×s	447.54	Joback Method
dvisc	0.0004775	Pa×s	494.47	Joback Method
dvisc	0.0002997	Pa×s	541.40	Joback Method
dvisc	0.0002026	Pa×s	588.33	Joback Method
dvisc	0.0001451	Pa×s	635.26	Joback Method
dvisc	0.0001088	Pa×s	682.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74339494&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume