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

Physical Properties

Property code	Value	Unit	Source
af	0.7079		Cheméo Relay (1.0)
hf	-645.00	kJ/mol	Cheméo Relay (1.0)
hfus	37.39	kJ/mol	Joback Method
hvap	80.72	kJ/mol	Cheméo Relay (1.0)
ie	10.26	eV	Cheméo Relay (1.0)
log10ws	-6.35		Cheméo Relay (1.0)
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	562.55	K	Cheméo Relay (1.0)
tc	759.21	K	Cheméo Relay (1.0)
tf	274.01	K	Cheméo Relay (1.0)
vc	0.895	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74339494&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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