Trichloroacetic acid, pentadecyl ester

Other names: Pentadecyl trichloroacetate
Inchi: InChI=1S/C17H31Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-16(21)17(18,19)20/h2
InchiKey: NKIOTTYRINVYJZ-UHFFFAOYSA-N
Formula: C17H31Cl3O2
SMILES: CCCCCCCCCCCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 373.79
CAS: 74339-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-174.61	kJ/mol	Joback Method
hf	-694.98	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	74.45	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	6.991		Crippen Method
mcvol	294.550	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	2271.00		NIST Webbook
tb	773.71	K	Joback Method
tc	961.69	K	Joback Method
tf	445.69	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.09	J/mol×K	773.71	Joback Method
cpg	849.11	J/mol×K	805.04	Joback Method
cpg	864.22	J/mol×K	836.37	Joback Method
cpg	878.48	J/mol×K	867.70	Joback Method
cpg	891.92	J/mol×K	899.03	Joback Method
cpg	904.58	J/mol×K	930.36	Joback Method
cpg	916.52	J/mol×K	961.69	Joback Method

dvisc	0.0010626	Pa×s	445.69	Joback Method
dvisc	0.0005051	Pa×s	500.36	Joback Method
dvisc	0.0002780	Pa×s	555.03	Joback Method
dvisc	0.0001703	Pa×s	609.70	Joback Method
dvisc	0.0001131	Pa×s	664.37	Joback Method
dvisc	0.0000799	Pa×s	719.04	Joback Method
dvisc	0.0000593	Pa×s	773.71	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=C74339530&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