2,2,2-Trichloroethyl pentadecanoate

Inchi: InChI=1S/C17H31Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16(21)22-15-17(18,19)20/h2
InchiKey: BZZHDMKALRSLCY-UHFFFAOYSA-N
Formula: C17H31Cl3O2
SMILES: CCCCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 373.79

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	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
rinpol	2276.00		NIST Webbook
rinpol	2278.00		NIST Webbook
ripol	2638.00		NIST Webbook
ripol	2666.00		NIST Webbook
ripol	2666.00		NIST Webbook
ripol	2682.00		NIST Webbook
ripol	2638.00		NIST Webbook
ripol	2646.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2670.00		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	904.58	J/mol×K	930.36	Joback Method
cpg	891.92	J/mol×K	899.03	Joback Method
cpg	878.48	J/mol×K	867.70	Joback Method
cpg	864.22	J/mol×K	836.37	Joback Method
cpg	849.11	J/mol×K	805.04	Joback Method
cpg	916.52	J/mol×K	961.69	Joback Method
dvisc	0.0000593	Pa×s	773.71	Joback Method
dvisc	0.0000799	Pa×s	719.04	Joback Method
dvisc	0.0001131	Pa×s	664.37	Joback Method
dvisc	0.0001703	Pa×s	609.70	Joback Method
dvisc	0.0002780	Pa×s	555.03	Joback Method
dvisc	0.0005051	Pa×s	500.36	Joback Method
dvisc	0.0010626	Pa×s	445.69	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30513&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

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