2,2,2-Trichloroethyl octadecanoate

Inchi: InChI=1S/C20H37Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19(24)25-18-20(21
InchiKey: LFXBJDVOZVVFHT-UHFFFAOYSA-N
Formula: C20H37Cl3O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 415.87

Physical Properties

Property code	Value	Unit	Source
gf	-149.35	kJ/mol	Joback Method
hf	-756.90	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	81.13	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	8.161		Crippen Method
mcvol	336.820	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2575.00		NIST Webbook
ripol	2980.00		NIST Webbook
ripol	2969.00		NIST Webbook
ripol	2980.00		NIST Webbook
ripol	2988.00		NIST Webbook
ripol	2975.00		NIST Webbook
ripol	2969.00		NIST Webbook
tb	842.35	K	Joback Method
tc	1034.98	K	Joback Method
tf	479.50	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1009.89	J/mol×K	842.35	Joback Method
cpg	1027.01	J/mol×K	874.46	Joback Method
cpg	1043.14	J/mol×K	906.56	Joback Method
cpg	1058.34	J/mol×K	938.67	Joback Method
cpg	1072.65	J/mol×K	970.77	Joback Method
cpg	1086.12	J/mol×K	1002.88	Joback Method
cpg	1098.81	J/mol×K	1034.98	Joback Method
dvisc	0.0007258	Pa×s	479.50	Joback Method
dvisc	0.0003345	Pa×s	539.98	Joback Method
dvisc	0.0001802	Pa×s	600.45	Joback Method
dvisc	0.0001087	Pa×s	660.92	Joback Method
dvisc	0.0000714	Pa×s	721.40	Joback Method
dvisc	0.0000500	Pa×s	781.88	Joback Method
dvisc	0.0000369	Pa×s	842.35	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30492&Units=SI

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