trichloroacetic acid, stearyl ester

Other names: Octadecyl trichloroacetate
Inchi: InChI=1S/C20H37Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-25-19(24)20(21
InchiKey: SHVKFBUBFSLWFV-UHFFFAOYSA-N
Formula: C20H37Cl3O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(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	2571.00		NIST Webbook
rinpol	2588.00		NIST Webbook
rinpol	2571.00		NIST Webbook
ripol	2987.00		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	1086.12	J/mol×K	1002.88	Joback Method
cpg	1072.65	J/mol×K	970.77	Joback Method
cpg	1058.34	J/mol×K	938.67	Joback Method
cpg	1043.14	J/mol×K	906.56	Joback Method

cpg	1027.01	J/mol×K	874.46	Joback Method
cpg	1098.81	J/mol×K	1034.98	Joback Method
dvisc	0.0000369	Pa×s	842.35	Joback Method
dvisc	0.0000500	Pa×s	781.88	Joback Method
dvisc	0.0000714	Pa×s	721.40	Joback Method
dvisc	0.0001087	Pa×s	660.92	Joback Method
dvisc	0.0001802	Pa×s	600.45	Joback Method
dvisc	0.0003345	Pa×s	539.98	Joback Method
dvisc	0.0007258	Pa×s	479.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R146231&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

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