Trichloroacetic acid, hexadecyl ester

Other names: Trichloroacetic acid, palmityl ester
Acetic acid, trichloro-, hexadecyl ester
Hexadecyl trichloroacetate
Inchi: InChI=1S/C18H33Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-17(22)18(19,20)21
InchiKey: CCFJXGUHYQBXDT-UHFFFAOYSA-N
Formula: C18H33Cl3O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 387.81
CAS: 74339-54-1

Physical Properties

Property code	Value	Unit	Source
gf	-166.19	kJ/mol	Joback Method
hf	-715.62	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	76.68	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	7.381		Crippen Method
mcvol	308.640	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2364.90		NIST Webbook
rinpol	2364.90		NIST Webbook
rinpol	2381.00		NIST Webbook
rinpol	2381.00		NIST Webbook
rinpol	2371.00		NIST Webbook
ripol	2788.00		NIST Webbook
ripol	2788.00		NIST Webbook
tb	796.59	K	Joback Method
tc	985.44	K	Joback Method
tf	456.96	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.14	J/mol×K	796.59	Joback Method
cpg	964.18	J/mol×K	953.96	Joback Method
cpg	951.25	J/mol×K	922.49	Joback Method
cpg	937.52	J/mol×K	891.01	Joback Method
cpg	922.96	J/mol×K	859.54	Joback Method
cpg	907.51	J/mol×K	828.06	Joback Method
cpg	976.37	J/mol×K	985.44	Joback Method
dvisc	0.0000507	Pa×s	796.59	Joback Method
dvisc	0.0000685	Pa×s	739.99	Joback Method
dvisc	0.0000972	Pa×s	683.38	Joback Method
dvisc	0.0001469	Pa×s	626.77	Joback Method
dvisc	0.0002411	Pa×s	570.17	Joback Method
dvisc	0.0004414	Pa×s	513.56	Joback Method
dvisc	0.0009387	Pa×s	456.96	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=C74339541&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