2,2,2-Trichloroethyl tetradecanoate

Inchi: InChI=1S/C16H29Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-15(20)21-14-16(17,18)19/h2-14
InchiKey: LROGLTHRRUHOKR-UHFFFAOYSA-N
Formula: C16H29Cl3O2
SMILES: CCCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 359.76

Physical Properties

Property code	Value	Unit	Source
gf	-183.03	kJ/mol	Joback Method
hf	-674.34	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	6.601		Crippen Method
mcvol	280.460	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2175.00		NIST Webbook
ripol	2544.00		NIST Webbook
ripol	2558.00		NIST Webbook
ripol	2582.00		NIST Webbook
ripol	2568.00		NIST Webbook
ripol	2565.00		NIST Webbook
ripol	2537.00		NIST Webbook
tb	750.83	K	Joback Method
tc	938.56	K	Joback Method
tf	434.42	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	776.02	J/mol×K	750.83	Joback Method
cpg	791.67	J/mol×K	782.12	Joback Method
cpg	806.45	J/mol×K	813.41	Joback Method
cpg	820.39	J/mol×K	844.69	Joback Method
cpg	833.54	J/mol×K	875.98	Joback Method
cpg	845.93	J/mol×K	907.27	Joback Method
cpg	857.60	J/mol×K	938.56	Joback Method
dvisc	0.0011988	Pa×s	434.42	Joback Method
dvisc	0.0005763	Pa×s	487.16	Joback Method
dvisc	0.0003196	Pa×s	539.89	Joback Method
dvisc	0.0001969	Pa×s	592.62	Joback Method
dvisc	0.0001313	Pa×s	645.36	Joback Method
dvisc	0.0000930	Pa×s	698.10	Joback Method
dvisc	0.0000692	Pa×s	750.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30531&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