2,2,2-Trichloroethyl hexanoate

Other names: Hexanoic acid, 2,2,2-trichloroethyl ester
Inchi: InChI=1S/C8H13Cl3O2/c1-2-3-4-5-7(12)13-6-8(9,10)11/h2-6H2,1H3
InchiKey: WGQPNMRSQVQUSL-UHFFFAOYSA-N
Formula: C8H13Cl3O2
SMILES: CCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 247.55

Physical Properties

Property code	Value	Unit	Source
gf	-250.39	kJ/mol	Joback Method
hf	-509.22	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	54.42	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.480		Crippen Method
mcvol	167.740	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1336.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1378.00		NIST Webbook
ripol	1739.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1761.00		NIST Webbook
tb	567.79	K	Joback Method
tc	769.47	K	Joback Method
tf	344.26	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.45	J/mol×K	567.79	Joback Method
cpg	413.95	J/mol×K	735.85	Joback Method
cpg	405.09	J/mol×K	702.24	Joback Method
cpg	395.65	J/mol×K	668.63	Joback Method
cpg	385.58	J/mol×K	635.02	Joback Method
cpg	374.85	J/mol×K	601.40	Joback Method
cpg	422.23	J/mol×K	769.47	Joback Method
dvisc	0.0002194	Pa×s	567.79	Joback Method
dvisc	0.0002876	Pa×s	530.53	Joback Method
dvisc	0.0003926	Pa×s	493.28	Joback Method
dvisc	0.0005639	Pa×s	456.02	Joback Method
dvisc	0.0008638	Pa×s	418.77	Joback Method
dvisc	0.0014383	Pa×s	381.51	Joback Method
dvisc	0.0026742	Pa×s	344.26	Joback Method

Sources

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=R19765&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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