2,2,2-Trichloroethyl octanoate

Other names: Octanoic acid, 2,2,2-trichloroethyl ester
Inchi: InChI=1S/C10H17Cl3O2/c1-2-3-4-5-6-7-9(14)15-8-10(11,12)13/h2-8H2,1H3
InchiKey: HSGDHOUWEKLJIE-UHFFFAOYSA-N
Formula: C10H17Cl3O2
SMILES: CCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 275.60

Physical Properties

Property code	Value	Unit	Source
gf	-233.55	kJ/mol	Joback Method
hf	-550.50	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	58.87	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.260		Crippen Method
mcvol	195.920	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1578.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1997.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1948.00		NIST Webbook
tb	613.55	K	Joback Method
tc	809.74	K	Joback Method

tf	366.80	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.10	J/mol×K	613.55	Joback Method
cpg	470.97	J/mol×K	646.25	Joback Method
cpg	483.09	J/mol×K	678.95	Joback Method
cpg	494.50	J/mol×K	711.65	Joback Method
cpg	505.23	J/mol×K	744.35	Joback Method
cpg	515.31	J/mol×K	777.04	Joback Method
cpg	524.77	J/mol×K	809.74	Joback Method
dvisc	0.0022618	Pa×s	366.80	Joback Method
dvisc	0.0011775	Pa×s	407.93	Joback Method
dvisc	0.0006909	Pa×s	449.05	Joback Method
dvisc	0.0004433	Pa×s	490.17	Joback Method
dvisc	0.0003047	Pa×s	531.30	Joback Method
dvisc	0.0002210	Pa×s	572.42	Joback Method
dvisc	0.0001674	Pa×s	613.55	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=R19961&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