

1-chlorooctyl trichloroacetate

Other names:	1-Octanol, 1-chloro, trichloroacetate
Inchi:	InChI=1S/C10H16Cl4O2/c1-2-3-4-5-6-7-8(11)16-9(15)10(12,13)14/h8H,2-7H2,1H3
InchiKey:	VLCBCOLHPTXRFH-UHFFFAOYSA-N
Formula:	C10H16Cl4O2
SMILES:	CCCCCCCC(Cl)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	310.05

Physical Properties

Property code	Value	Unit	Source
gf	-247.92	kJ/mol	Joback Method
hf	-571.52	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.825		Crippen Method
mcvol	208.160	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1624.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1624.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2057.00		NIST Webbook
ripol	2023.00		NIST Webbook
tb	650.54	K	Joback Method
tc	854.25	K	Joback Method
tf	381.72	K	Joback Method
vc	0.798	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	484.42	J/molxK	650.54	Joback Method
cpg	496.64	J/molxK	684.49	Joback Method
cpg	508.09	J/molxK	718.44	Joback Method
cpg	518.80	J/molxK	752.39	Joback Method
cpg	528.80	J/molxK	786.35	Joback Method
cpg	538.14	J/molxK	820.30	Joback Method
cpg	546.84	J/molxK	854.25	Joback Method
dvisc	0.0022272	Paxs	381.72	Joback Method
dvisc	0.0010938	Paxs	426.52	Joback Method
dvisc	0.0006150	Paxs	471.33	Joback Method
dvisc	0.0003821	Paxs	516.13	Joback Method
dvisc	0.0002562	Paxs	560.93	Joback Method
dvisc	0.0001822	Paxs	605.74	Joback Method
dvisc	0.0001358	Paxs	650.54	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=R112104&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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