

3-chloropentyl trichloroacetate

Other names:	1-Pentanol, 3-chloro, trichloroacetate
Inchi:	InChI=1S/C7H10Cl4O2/c1-2-5(8)3-4-13-6(12)7(9,10)11/h5H,2-4H2,1H3
InchiKey:	XNBBFBOMOPSUMI-UHFFFAOYSA-N
Formula:	C7H10Cl4O2
SMILES:	CCC(Cl)CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	267.96

Physical Properties

Property code	Value	Unit	Source
gf	-273.18	kJ/mol	Joback Method
hf	-509.60	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	56.19	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.307		Crippen Method
mcvol	165.890	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
ripol	1382.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1437.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	2013.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1978.00		NIST Webbook
tb	581.90	K	Joback Method
tc	795.32	K	Joback Method
tf	347.91	K	Joback Method
vc	0.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	342.31	J/molxK	581.90	Joback Method
cpg	352.30	J/molxK	617.47	Joback Method
cpg	361.62	J/molxK	653.04	Joback Method
cpg	370.28	J/molxK	688.61	Joback Method
cpg	378.32	J/molxK	724.18	Joback Method
cpg	385.77	J/molxK	759.75	Joback Method
cpg	392.66	J/molxK	795.32	Joback Method
dvisc	0.0029975	Paxs	347.91	Joback Method
dvisc	0.0015388	Paxs	386.91	Joback Method
dvisc	0.0008926	Paxs	425.91	Joback Method
dvisc	0.0005673	Paxs	464.90	Joback Method
dvisc	0.0003867	Paxs	503.90	Joback Method
dvisc	0.0002785	Paxs	542.90	Joback Method
dvisc	0.0002097	Paxs	581.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R112426&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

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