

1-chlorohexyl trichloroacetate

Other names:	1-Hexanol, 1-chloro, trichloroacetate
Inchi:	InChI=1S/C8H12Cl4O2/c1-2-3-4-5-6(9)14-7(13)8(10,11)12/h6H,2-5H2,1H3
InchiKey:	AOVWSGPNPYRTMSO-UHFFFAOYSA-N
Formula:	C8H12Cl4O2
SMILES:	CCCCCC(Cl)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	281.99

Physical Properties

Property code	Value	Unit	Source
gf	-264.76	kJ/mol	Joback Method
hf	-530.24	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	58.41	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.045		Crippen Method
mcvol	179.980	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1429.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1829.00		NIST Webbook
tb	604.78	K	Joback Method
tc	814.70	K	Joback Method
tf	359.18	K	Joback Method
vc	0.686	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.10	J/molxK	604.78	Joback Method
cpg	435.44	J/molxK	779.72	Joback Method
cpg	427.28	J/molxK	744.73	Joback Method
cpg	418.49	J/molxK	709.74	Joback Method
cpg	409.06	J/molxK	674.75	Joback Method
cpg	398.94	J/molxK	639.77	Joback Method
cpg	443.01	J/molxK	814.70	Joback Method
dvisc	0.0001819	Paxs	604.78	Joback Method
dvisc	0.0002425	Paxs	563.85	Joback Method
dvisc	0.0003382	Paxs	522.91	Joback Method
dvisc	0.0004991	Paxs	481.98	Joback Method
dvisc	0.0007916	Paxs	441.05	Joback Method
dvisc	0.0013799	Paxs	400.11	Joback Method
dvisc	0.0027302	Paxs	359.18	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=R111903&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
ripol:	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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