

3-chloroheptyl trichloroacetate

Other names:	1-Heptanol, 3-chloro, trichloroacetate
Inchi:	InChI=1S/C9H14Cl4O2/c1-2-3-4-7(10)5-6-15-8(14)9(11,12)13/h7H,2-6H2,1H3
InchiKey:	GBDMMAMPWAWARJ-UHFFFAOYSA-N
Formula:	C9H14Cl4O2
SMILES:	CCCCCC(Cl)CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	296.02

Physical Properties

Property code	Value	Unit	Source
gf	-256.34	kJ/mol	Joback Method
hf	-550.88	kJ/mol	Joback Method
hfus	27.70	kJ/mol	Joback Method
hvap	60.64	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.088		Crippen Method
mcvol	194.070	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1599.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2162.00		NIST Webbook
tb	627.66	K	Joback Method
tc	834.33	K	Joback Method
tf	370.45	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.50	J/molxK	627.66	Joback Method

cpg	447.08	J/molxK	662.11	Joback Method
cpg	457.91	J/molxK	696.55	Joback Method
cpg	468.02	J/molxK	731.00	Joback Method
cpg	477.45	J/molxK	765.44	Joback Method
cpg	486.24	J/molxK	799.89	Joback Method
cpg	494.41	J/molxK	834.33	Joback Method
dvisc	0.0024724	Paxs	370.45	Joback Method
dvisc	0.0012314	Paxs	413.32	Joback Method
dvisc	0.0006991	Paxs	456.19	Joback Method
dvisc	0.0004375	Paxs	499.05	Joback Method
dvisc	0.0002948	Paxs	541.92	Joback Method
dvisc	0.0002105	Paxs	584.79	Joback Method
dvisc	0.0001574	Paxs	627.66	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=R111730&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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