6-chloroheptyl trichloroacetate

Other names:	1-Heptanol, 6-chloro, trichloroacetate
Inchi:	InChI=1S/C9H14Cl4O2/c1-7(10)5-3-2-4-6-15-8(14)9(11,12)13/h7H,2-6H2,1H3
InchiKey:	IBGLZKHCYPMZSV-UHFFFAOYSA-N
Formula:	C9H14Cl4O2
SMILES:	CC(Cl)CCCCCOC(=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	1659.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1679.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2301.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2285.00		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/mol×K	627.66	Joback Method
cpg	486.24	J/mol×K	799.89	Joback Method
cpg	477.45	J/mol×K	765.44	Joback Method
cpg	468.02	J/mol×K	731.00	Joback Method
cpg	457.91	J/mol×K	696.55	Joback Method
cpg	447.08	J/mol×K	662.11	Joback Method
cpg	494.41	J/mol×K	834.33	Joback Method
dvisc	0.0001574	Pa×s	627.66	Joback Method
dvisc	0.0002105	Pa×s	584.79	Joback Method
dvisc	0.0002948	Pa×s	541.92	Joback Method
dvisc	0.0004375	Pa×s	499.05	Joback Method
dvisc	0.0006991	Pa×s	456.19	Joback Method
dvisc	0.0012314	Pa×s	413.32	Joback Method
dvisc	0.0024724	Pa×s	370.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R111829&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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