Trichloroacetic acid, 6-chlorohexyl ester

Other names:	6-chlorohexyl trichloroacetate
	1-Hexanol, 6-chloro, trichloroacetate
Inchi:	InChI=1S/C8H12Cl4O2/c9-5-3-1-2-4-6-14-7(13)8(10,11)12/h1-6H2
InchiKey:	SCWOHXIWHLOZJV-UHFFFAOYSA-N
Formula:	C8H12Cl4O2
SMILES:	O=C(OCCCCCCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	281.99

Physical Properties

Property code	Value	Unit	Source
gf	-262.32	kJ/mol	Joback Method
hf	-524.96	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	58.80	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.699		Crippen Method
mcvol	179.980	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1638.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2258.00		NIST Webbook
tb	605.22	K	Joback Method
tc	811.00	K	Joback Method
tf	374.18	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.62	J/mol×K	605.22	Joback Method
cpg	434.01	J/mol×K	776.70	Joback Method
cpg	425.97	J/mol×K	742.41	Joback Method
cpg	417.34	J/mol×K	708.11	Joback Method
cpg	408.10	J/mol×K	673.81	Joback Method
cpg	398.20	J/mol×K	639.52	Joback Method
cpg	441.49	J/mol×K	811.00	Joback Method
dvisc	0.0001948	Pa×s	605.22	Joback Method
dvisc	0.0002539	Pa×s	566.71	Joback Method
dvisc	0.0003439	Pa×s	528.21	Joback Method
dvisc	0.0004884	Pa×s	489.70	Joback Method
dvisc	0.0007367	Pa×s	451.19	Joback Method
dvisc	0.0011996	Pa×s	412.69	Joback Method
dvisc	0.0021596	Pa×s	374.18	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U330892&Units=SI
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

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