3-chlorohexyl trichloroacetate

Other names: 1-Hexanol, 3-chloro, trichloroacetate
Inchi: InChI=1S/C8H12Cl4O2/c1-2-3-6(9)4-5-14-7(13)8(10,11)12/h6H,2-5H2,1H3
InchiKey: HXOCGLLNDYVEHJ-UHFFFAOYSA-N
Formula: C8H12Cl4O2
SMILES: CCCC(Cl)CCOC(=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	-3.86		Crippen Method
logp	3.697		Crippen Method
mcvol	179.980	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1532.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1467.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2061.00		NIST Webbook
tb	604.78	K	Joback Method
tc	814.70	K	Joback Method
tf	359.18	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.10	J/mol×K	604.78	Joback Method

cpg	435.44	J/mol×K	779.72	Joback Method
cpg	427.28	J/mol×K	744.73	Joback Method
cpg	418.49	J/mol×K	709.74	Joback Method
cpg	409.06	J/mol×K	674.75	Joback Method
cpg	398.94	J/mol×K	639.77	Joback Method
cpg	443.01	J/mol×K	814.70	Joback Method
dvisc	0.0001819	Pa×s	604.78	Joback Method
dvisc	0.0002425	Pa×s	563.85	Joback Method
dvisc	0.0003382	Pa×s	522.91	Joback Method
dvisc	0.0004991	Pa×s	481.98	Joback Method
dvisc	0.0007916	Pa×s	441.05	Joback Method
dvisc	0.0013799	Pa×s	400.11	Joback Method
dvisc	0.0027302	Pa×s	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=R111963&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
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