8-chlorooctyl trichloroacetate

Other names: 1-Octanol, 8-chloro, trichloroacetate
Inchi: InChI=1S/C10H16Cl4O2/c11-7-5-3-1-2-4-6-8-16-9(15)10(12,13)14/h1-8H2
InchiKey: QQGWBYRTWYPUTG-UHFFFAOYSA-N
Formula: C10H16Cl4O2
SMILES: O=C(OCCCCCCCCCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 310.05

Physical Properties

Property code	Value	Unit	Source
gf	-245.48	kJ/mol	Joback Method
hf	-566.24	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	63.25	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.479		Crippen Method
mcvol	208.160	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1812.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1812.00		NIST Webbook
ripol	2472.00		NIST Webbook
ripol	2491.00		NIST Webbook
ripol	2446.00		NIST Webbook
tb	650.98	K	Joback Method
tc	851.05	K	Joback Method
tf	396.72	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.91	J/mol×K	650.98	Joback Method

cpg	495.88	J/mol×K	684.33	Joback Method
cpg	507.11	J/mol×K	717.67	Joback Method
cpg	517.63	J/mol×K	751.02	Joback Method
cpg	527.48	J/mol×K	784.36	Joback Method
cpg	536.70	J/mol×K	817.71	Joback Method
cpg	545.31	J/mol×K	851.05	Joback Method
dvisc	0.0017922	Pa×s	396.72	Joback Method
dvisc	0.0009647	Pa×s	439.10	Joback Method
dvisc	0.0005791	Pa×s	481.47	Joback Method
dvisc	0.0003775	Pa×s	523.85	Joback Method
dvisc	0.0002624	Pa×s	566.23	Joback Method
dvisc	0.0001919	Pa×s	608.60	Joback Method
dvisc	0.0001461	Pa×s	650.98	Joback Method

Sources

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=R112317&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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