7-chloroheptyl trichloroacetate

Other names: 1-Heptanol, 7-chloro, trichloroacetate
Inchi: InChI=1S/C9H14Cl4O2/c10-6-4-2-1-3-5-7-15-8(14)9(11,12)13/h1-7H2
InchiKey: QKQBBAIFCVZRFD-UHFFFAOYSA-N
Formula: C9H14Cl4O2
SMILES: O=C(OCCCCCCCCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 296.02

Physical Properties

Property code	Value	Unit	Source
gf	-253.90	kJ/mol	Joback Method
hf	-545.60	kJ/mol	Joback Method
hfus	31.23	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	4.089		Crippen Method
mcvol	194.070	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1745.00		NIST Webbook
ripol	2354.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2393.00		NIST Webbook
tb	628.10	K	Joback Method
tc	830.88	K	Joback Method
tf	385.45	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.00	J/mol×K	628.10	Joback Method
cpg	446.32	J/mol×K	661.90	Joback Method

cpg	456.93	J/mol×K	695.69	Joback Method
cpg	466.85	J/mol×K	729.49	Joback Method
cpg	476.13	J/mol×K	763.29	Joback Method
cpg	484.80	J/mol×K	797.08	Joback Method
cpg	492.88	J/mol×K	830.88	Joback Method
dvisc	0.0019729	Pa×s	385.45	Joback Method
dvisc	0.0010784	Pa×s	425.89	Joback Method
dvisc	0.0006545	Pa×s	466.33	Joback Method
dvisc	0.0004302	Pa×s	506.77	Joback Method
dvisc	0.0003009	Pa×s	547.22	Joback Method
dvisc	0.0002211	Pa×s	587.66	Joback Method
dvisc	0.0001690	Pa×s	628.10	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=R111854&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