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	1745.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1736.00		NIST Webbook
ripol	2393.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2354.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R111854&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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