Trichloroacetic acid, pentyl ester

Other names: Pentyl trichloroacetate
Inchi: InChI=1S/C7H11Cl3O2/c1-2-3-4-5-12-6(11)7(8,9)10/h2-5H2,1H3
InchiKey: LZJOVWVTJGLPFN-UHFFFAOYSA-N
Formula: C7H11Cl3O2
SMILES: CCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 233.52
CAS: 33972-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-258.81	kJ/mol	Joback Method
hf	-488.58	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.090		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1240.20		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1216.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1668.00		NIST Webbook
tb	544.91	K	Joback Method
tc	749.61	K	Joback Method
tf	332.99	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.66	J/mol×K	544.91	Joback Method
cpg	329.17	J/mol×K	579.03	Joback Method
cpg	339.04	J/mol×K	613.14	Joback Method
cpg	348.30	J/mol×K	647.26	Joback Method
cpg	356.97	J/mol×K	681.38	Joback Method
cpg	365.08	J/mol×K	715.49	Joback Method
cpg	372.65	J/mol×K	749.61	Joback Method
dvisc	0.0028764	Pa×s	332.99	Joback Method
dvisc	0.0015745	Pa×s	368.31	Joback Method
dvisc	0.0009578	Pa×s	403.63	Joback Method
dvisc	0.0006311	Pa×s	438.95	Joback Method
dvisc	0.0004425	Pa×s	474.27	Joback Method
dvisc	0.0003259	Pa×s	509.59	Joback Method
dvisc	0.0002498	Pa×s	544.91	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=C33972815&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