Trichloroacetic acid, 2-pentyl ester

Other names: Acetic acid, trichloro, 1-methylbutyl ester
Inchi: InChI=1S/C7H11Cl3O2/c1-3-4-5(2)12-6(11)7(8,9)10/h5H,3-4H2,1-2H3
InchiKey: GKGUCQJRCNVBMU-UHFFFAOYSA-N
Formula: C7H11Cl3O2
SMILES: CCCC(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 233.52
CAS: 78031-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-261.25	kJ/mol	Joback Method
hf	-493.86	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.088		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1469.00		NIST Webbook
tb	544.47	K	Joback Method
tc	753.60	K	Joback Method
tf	317.99	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.04	J/mol×K	544.47	Joback Method
cpg	329.84	J/mol×K	579.32	Joback Method
cpg	339.96	J/mol×K	614.18	Joback Method
cpg	349.44	J/mol×K	649.03	Joback Method

cpg	358.30	J/mol×K	683.89	Joback Method
cpg	366.56	J/mol×K	718.74	Joback Method
cpg	374.25	J/mol×K	753.60	Joback Method
dvisc	0.0038109	Pa×s	317.99	Joback Method
dvisc	0.0018721	Pa×s	355.74	Joback Method
dvisc	0.0010540	Pa×s	393.48	Joback Method
dvisc	0.0006562	Pa×s	431.23	Joback Method
dvisc	0.0004410	Pa×s	468.98	Joback Method
dvisc	0.0003144	Pa×s	506.72	Joback Method
dvisc	0.0002349	Pa×s	544.47	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78031353&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

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