Pentanoic acid, 4-methyl, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C8H13Cl3O2/c1-6(2)3-4-7(12)13-5-8(9,10)11/h6H,3-5H2,1-2H3
InchiKey: GGNAUVDISWUXRK-UHFFFAOYSA-N
Formula: C8H13Cl3O2
SMILES: CC(C)CCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 247.55

Physical Properties

Property code	Value	Unit	Source
gf	-252.83	kJ/mol	Joback Method
hf	-514.50	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	54.03	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.336		Crippen Method
mcvol	167.740	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
tb	567.35	K	Joback Method
tc	773.22	K	Joback Method
tf	329.26	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.86	J/mol×K	567.35	Joback Method
cpg	375.55	J/mol×K	601.66	Joback Method
cpg	386.53	J/mol×K	635.97	Joback Method
cpg	396.83	J/mol×K	670.29	Joback Method
cpg	406.46	J/mol×K	704.60	Joback Method
cpg	415.47	J/mol×K	738.91	Joback Method
cpg	423.87	J/mol×K	773.22	Joback Method
dvisc	0.0035039	Pa×s	329.26	Joback Method

dvisc	0.0016943	Pa×s	368.94	Joback Method
dvisc	0.0009435	Pa×s	408.62	Joback Method
dvisc	0.0005827	Pa×s	448.31	Joback Method
dvisc	0.0003893	Pa×s	487.99	Joback Method
dvisc	0.0002763	Pa×s	527.67	Joback Method
dvisc	0.0002058	Pa×s	567.35	Joback Method

Sources

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=R20017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume