Trichloroacetic acid, 3-methylphenyl ester

Inchi: InChI=1S/C9H7Cl3O2/c1-6-3-2-4-7(5-6)14-8(13)9(10,11)12/h2-5H,1H3
InchiKey: WEXLTVMJHWNNTN-UHFFFAOYSA-N
Formula: C9H7Cl3O2
SMILES: Cc1cccc(OC(=O)C(Cl)(Cl)Cl)c1
Mol. weight [g/mol]: 253.51

Physical Properties

Property code	Value	Unit	Source
gf	-139.19	kJ/mol	Joback Method
hf	-304.80	kJ/mol	Joback Method
hfus	20.68	kJ/mol	Joback Method
hvap	59.58	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.271		Crippen Method
mcvol	158.070	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
tb	622.33	K	Joback Method
tc	866.50	K	Joback Method
tf	394.47	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.91	J/mol×K	622.33	Joback Method
cpg	340.21	J/mol×K	663.03	Joback Method
cpg	349.60	J/mol×K	703.72	Joback Method
cpg	358.16	J/mol×K	744.42	Joback Method
cpg	365.92	J/mol×K	785.11	Joback Method
cpg	372.94	J/mol×K	825.81	Joback Method
cpg	379.27	J/mol×K	866.50	Joback Method
dvisc	0.0014971	Pa×s	394.47	Joback Method

dvisc	0.0009046	Pa×s	432.45	Joback Method
dvisc	0.0005929	Pa×s	470.42	Joback Method
dvisc	0.0004140	Pa×s	508.40	Joback Method
dvisc	0.0003038	Pa×s	546.38	Joback Method
dvisc	0.0002321	Pa×s	584.35	Joback Method
dvisc	0.0001833	Pa×s	622.33	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=U307719&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume