Trichloroacetic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C10H9Cl3O2/c1-6-3-7(2)5-8(4-6)15-9(14)10(11,12)13/h3-5H,1-2H3
InchiKey: RKKOPRPERWQZIH-UHFFFAOYSA-N
Formula: C10H9Cl3O2
SMILES: Cc1cc(C)cc(OC(=O)C(Cl)(Cl)Cl)c1
Mol. weight [g/mol]: 267.54

Physical Properties

Property code	Value	Unit	Source
gf	-140.40	kJ/mol	Joback Method
hf	-336.91	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.579		Crippen Method
mcvol	172.160	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
tb	650.19	K	Joback Method
tc	890.08	K	Joback Method
tf	418.26	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.31	J/mol×K	650.19	Joback Method
cpg	386.22	J/mol×K	690.17	Joback Method
cpg	396.26	J/mol×K	730.15	Joback Method
cpg	405.45	J/mol×K	770.13	Joback Method
cpg	413.86	J/mol×K	810.11	Joback Method
cpg	421.53	J/mol×K	850.10	Joback Method
cpg	428.50	J/mol×K	890.08	Joback Method
dvisc	0.0011373	Pa×s	418.26	Joback Method

dvisc	0.0007134	Pa×s	456.92	Joback Method
dvisc	0.0004813	Pa×s	495.57	Joback Method
dvisc	0.0003437	Pa×s	534.23	Joback Method
dvisc	0.0002569	Pa×s	572.88	Joback Method
dvisc	0.0001992	Pa×s	611.54	Joback Method
dvisc	0.0001592	Pa×s	650.19	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=U307721&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