Trichloroacetic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C9H7Cl3O3/c1-14-6-2-4-7(5-3-6)15-8(13)9(10,11)12/h2-5H,1H3
InchiKey: MMIXCSCJXHTNAC-UHFFFAOYSA-N
Formula: C9H7Cl3O3
SMILES: COc1ccc(OC(=O)C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 269.51

Physical Properties

Property code	Value	Unit	Source
gf	-244.19	kJ/mol	Joback Method
hf	-437.02	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.971		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1637.00		NIST Webbook
tb	644.75	K	Joback Method
tc	885.06	K	Joback Method
tf	416.70	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.90	J/mol×K	644.75	Joback Method
cpg	362.02	J/mol×K	684.80	Joback Method
cpg	371.29	J/mol×K	724.85	Joback Method
cpg	379.74	J/mol×K	764.91	Joback Method
cpg	387.40	J/mol×K	804.96	Joback Method
cpg	394.30	J/mol×K	845.01	Joback Method
cpg	400.47	J/mol×K	885.06	Joback Method
dvisc	0.0010679	Pa×s	416.70	Joback Method
dvisc	0.0006619	Pa×s	454.71	Joback Method

dvisc	0.0004416	Pa×s	492.72	Joback Method
dvisc	0.0003122	Pa×s	530.73	Joback Method
dvisc	0.0002312	Pa×s	568.73	Joback Method
dvisc	0.0001778	Pa×s	606.74	Joback Method
dvisc	0.0001410	Pa×s	644.75	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=U307722&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