Trichloroacetic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C8H4Cl4O2/c9-5-1-3-6(4-2-5)14-7(13)8(10,11)12/h1-4H
InchiKey: UAMJIPWXLGMBPW-UHFFFAOYSA-N
Formula: C8H4Cl4O2
SMILES: O=C(Oc1ccc(Cl)cc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 273.93

Physical Properties

Property code	Value	Unit	Source
gf	-159.54	kJ/mol	Joback Method
hf	-299.90	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.616		Crippen Method
mcvol	156.220	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1551.00		NIST Webbook
tb	636.88	K	Joback Method
tc	889.58	K	Joback Method
tf	413.12	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.35	J/mol×K	636.88	Joback Method
cpg	338.08	J/mol×K	847.46	Joback Method
cpg	332.79	J/mol×K	805.34	Joback Method
cpg	326.82	J/mol×K	763.23	Joback Method
cpg	320.14	J/mol×K	721.11	Joback Method
cpg	312.67	J/mol×K	679.00	Joback Method
cpg	342.76	J/mol×K	889.58	Joback Method
dvisc	0.0001871	Pa×s	636.88	Joback Method
dvisc	0.0002351	Pa×s	599.59	Joback Method

dvisc	0.0003046	Pa×s	562.29	Joback Method
dvisc	0.0004093	Pa×s	525.00	Joback Method
dvisc	0.0005755	Pa×s	487.71	Joback Method
dvisc	0.0008563	Pa×s	450.41	Joback Method
dvisc	0.0013686	Pa×s	413.12	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=U307720&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