Dichloroacetic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C8H5Cl3O2/c9-5-1-3-6(4-2-5)13-8(12)7(10)11/h1-4,7H
InchiKey: XBXQIOFECZDDPP-UHFFFAOYSA-N
Formula: C8H5Cl3O2
SMILES: O=C(Oc1ccc(Cl)cc1)C(Cl)Cl
Mol. weight [g/mol]: 239.48

Physical Properties

Property code	Value	Unit	Source
gf	-152.89	kJ/mol	Joback Method
hf	-280.69	kJ/mol	Joback Method
hfus	21.98	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.049		Crippen Method
mcvol	143.980	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	602.24	K	Joback Method
tc	841.79	K	Joback Method
tf	365.78	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.21	J/mol×K	602.24	Joback Method
cpg	290.36	J/mol×K	642.17	Joback Method
cpg	298.82	J/mol×K	682.09	Joback Method
cpg	306.60	J/mol×K	722.02	Joback Method
cpg	313.71	J/mol×K	761.94	Joback Method
cpg	320.18	J/mol×K	801.87	Joback Method
cpg	326.02	J/mol×K	841.79	Joback Method
dvisc	0.0017930	Pa×s	365.78	Joback Method

dvisc	0.0010631	Pa×s	405.19	Joback Method
dvisc	0.0006915	Pa×s	444.60	Joback Method
dvisc	0.0004824	Pa×s	484.01	Joback Method
dvisc	0.0003553	Pa×s	523.42	Joback Method
dvisc	0.0002731	Pa×s	562.83	Joback Method
dvisc	0.0002173	Pa×s	602.24	Joback Method

Sources

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=U307584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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