Dichloroacetic acid, 3-methylphenyl ester

Inchi: InChI=1S/C9H8Cl2O2/c1-6-3-2-4-7(5-6)13-9(12)8(10)11/h2-5,8H,1H3
InchiKey: PIRXAVOHMRJPRX-UHFFFAOYSA-N
Formula: C9H8Cl2O2
SMILES: Cc1cccc(OC(=O)C(Cl)Cl)c1
Mol. weight [g/mol]: 219.06

Physical Properties

Property code	Value	Unit	Source
gf	-132.54	kJ/mol	Joback Method
hf	-285.59	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.704		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1405.00		NIST Webbook
tb	587.69	K	Joback Method
tc	818.84	K	Joback Method
tf	347.13	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.59	J/mol×K	587.69	Joback Method
cpg	315.62	J/mol×K	626.22	Joback Method
cpg	325.90	J/mol×K	664.74	Joback Method
cpg	335.46	J/mol×K	703.27	Joback Method
cpg	344.32	J/mol×K	741.79	Joback Method
cpg	352.48	J/mol×K	780.32	Joback Method
cpg	359.97	J/mol×K	818.84	Joback Method
dvisc	0.0019276	Pa×s	347.13	Joback Method
dvisc	0.0010973	Pa×s	387.22	Joback Method

dvisc	0.0006944	Pa×s	427.32	Joback Method
dvisc	0.0004752	Pa×s	467.41	Joback Method
dvisc	0.0003454	Pa×s	507.50	Joback Method
dvisc	0.0002630	Pa×s	547.60	Joback Method
dvisc	0.0002078	Pa×s	587.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307583&Units=SI
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

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