2-Chlorobenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C13H5Cl5O2/c14-7-4-2-1-3-6(7)13(19)20-12-9(16)5-8(15)10(17)11(12)18/h1-5

InchiKey: UVQZZJAUBHJDGR-UHFFFAOYSA-N

Formula: C13H5Cl5O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccccc1Cl

Mol. weight [g/mol]: 370.44

Physical Properties

Property code	Value	Unit	Source
gf	-58.32	kJ/mol	Joback Method
hf	-219.44	kJ/mol	Joback Method
hfus	39.34	kJ/mol	Joback Method
hvap	83.47	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.173		Crippen Method
mcvol	215.150	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	838.54	K	Joback Method
tc	1100.44	K	Joback Method
tf	573.47	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.03	J/mol×K	838.54	Joback Method
cpg	469.93	J/mol×K	882.19	Joback Method
cpg	476.89	J/mol×K	925.84	Joback Method
cpg	482.94	J/mol×K	969.49	Joback Method
cpg	488.09	J/mol×K	1013.14	Joback Method
cpg	492.37	J/mol×K	1056.79	Joback Method
cpg	495.82	J/mol×K	1100.44	Joback Method
dvisc	0.0004360	Pa×s	573.47	Joback Method

dvisc	0.0003164	Pa×s	617.65	Joback Method
dvisc	0.0002397	Pa×s	661.83	Joback Method
dvisc	0.0001880	Pa×s	706.01	Joback Method
dvisc	0.0001517	Pa×s	750.18	Joback Method
dvisc	0.0001254	Pa×s	794.36	Joback Method
dvisc	0.0001057	Pa×s	838.54	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=U360529&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