

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

Inchi:	InChI=1S/C13H5Cl5O2/c14-7-3-1-6(2-4-7)13(19)20-12-9(16)5-8(15)10(17)11(12)18/h1-5
InchiKey:	CNOJGFZKPMMGQU-UHFFFAOYSA-N
Formula:	C13H5Cl5O2
SMILES:	O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccc(Cl)cc1
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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.03	J/molxK	838.54	Joback Method
cpg	469.93	J/molxK	882.19	Joback Method
cpg	476.89	J/molxK	925.84	Joback Method
cpg	482.94	J/molxK	969.49	Joback Method
cpg	488.09	J/molxK	1013.14	Joback Method
cpg	492.37	J/molxK	1056.79	Joback Method
cpg	495.82	J/molxK	1100.44	Joback Method
dvisc	0.0004360	Paxs	573.47	Joback Method
dvisc	0.0003164	Paxs	617.65	Joback Method

dvisc	0.0002397	Paxs	661.83	Joback Method
dvisc	0.0001880	Paxs	706.01	Joback Method
dvisc	0.0001517	Paxs	750.18	Joback Method
dvisc	0.0001254	Paxs	794.36	Joback Method
dvisc	0.0001057	Paxs	838.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U354631&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

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