

Dibenzofuran, 1,2,3,4-tetrachloro

Other names:	1,2,3,4-tetrachlorodibenzofuran
Inchi:	InChI=1S/C12H4Cl4O/c13-8-7-5-3-1-2-4-6(5)17-12(7)11(16)10(15)9(8)14/h1-4H
InchiKey:	AETAPIFVELRIDN-UHFFFAOYSA-N
Formula:	C12H4Cl4O
SMILES:	Clc1c(Cl)c(Cl)c2c(oc3ccccc32)c1Cl
Mol. weight [g/mol]:	305.97
CAS:	24478-72-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.55		Crippen Method
logp	6.200		Crippen Method
mcvol	176.390	ml/mol	McGowan Method
rinpol	2318.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2318.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	118.50	kJ/mol	363.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24478726&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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