Dibenzofuran, 1,3,4,6,8-pentachloro

Inchi: InChI=1S/C12H3Cl5O/c13-4-1-5-9-6(14)3-7(15)10(17)12(9)18-11(5)8(16)2-4/h1-3H
InchiKey: COKIAYPRHYHYCH-UHFFFAOYSA-N
Formula: C12H3Cl5O
SMILES: Clc1cc(Cl)c2oc3c(Cl)c(Cl)cc(Cl)c3c2c1
Mol. weight [g/mol]: 340.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.24		Crippen Method
logp	6.853		Crippen Method
mcvol	188.630	ml/mol	McGowan Method
rinpol	2404.00		NIST Webbook
rinpol	2418.00		NIST Webbook
rinpol	2404.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R48695&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/50-875-5/Dibenzofuran-1-3-4-6-8-pentachloro.pdf

Generated by Cheméo on 2025-12-24 22:24:13.804550977 +0000 UTC m=+6363251.334591641.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.