6-methyl-1,3-dichlorodibenzofuran

Inchi: InChI=1S/C13H8Cl2O/c1-7-3-2-4-9-12-10(15)5-8(14)6-11(12)16-13(7)9/h2-6H,1H3
InchiKey: GGFSEMBFVHJMCB-UHFFFAOYSA-N
Formula: C13H8Cl2O
SMILES: Cc1cccc2c1oc1cc(Cl)cc(Cl)c12
Mol. weight [g/mol]: 251.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.66		Crippen Method
logp	5.201		Crippen Method
mcvol	166.000	ml/mol	McGowan Method
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R173401&Units=SI

Legend

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

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