Dichlorophen, O,O'-di(2-furoyl)-

Inchi: InChI=1S/C23H14Cl2O6/c24-16-5-7-18(30-22(26)20-3-1-9-28-20)14(12-16)11-15-13-17(
InchiKey: RZMVCQXVJKGWDH-UHFFFAOYSA-N
Formula: C23H14Cl2O6
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1ccco1)c1ccco1
Mol. weight [g/mol]: 457.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.58		Crippen Method
logp	6.209		Crippen Method
mcvol	299.590	ml/mol	McGowan Method
rinpol	3365.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U355178&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