

pyrazoxyfen

Other names:	Ethanone, 2-[[4-(2,4-dichlorobenzoyl)-1,3-dimethyl-1H-pyrazol-5-yl]oxy]-1-phenyl-
Inchi:	InChI=1S/C20H16Cl2N2O3/c1-12-18(19(26)15-9-8-14(21)10-16(15)22)20(24(2)23-12)27
InchiKey:	FKERUJTUOYLBKB-UHFFFAOYSA-N
Formula:	C20H16Cl2N2O3
SMILES:	<chem>Cc1nn(C)c(OCC(=O)c2ccccc2)c1C(=O)c1ccc(Cl)cc1Cl</chem>
Mol. weight [g/mol]:	403.26
CAS:	71561-11-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	4.528		Crippen Method
mcvol	279.130	ml/mol	McGowan Method
rinsol	3004.00		NIST Webbook
rinsol	3004.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71561110&Units=SI
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

Legend

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

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