

Phellopterin

Inchi:	InChI=1S/C17H16O5/c1-10(2)6-8-21-17-15-12(7-9-20-15)14(19-3)11-4-5-13(18)22-16(1)
InchiKey:	BMLZFLQMBMYVHG-UHFFFAOYSA-N
Formula:	C17H16O5
SMILES:	COc1c2ccoc2c(OCC=C(C)C)c2oc(=O)ccc12
Mol. weight [g/mol]:	300.31
CAS:	2543-94-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.74		Crippen Method
logp	3.893		Crippen Method
mcvol	217.060	ml/mol	McGowan Method

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=C2543944&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/13-998-0/Phellopterin.pdf>

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