

WARFARIN METHYLATED

Inchi: InChI=1S/C20H18O4/c1-13(21)12-16(14-8-4-3-5-9-14)18-19(23-2)15-10-6-7-11-17(15)24
InchiKey: FGAWENWBTHQLEE-UHFFFAOYSA-N
Formula: C20H18O4
SMILES: COc1c(C(CC(C)=O)c2ccccc2)c(=O)oc2ccccc12
Mol. weight [g/mol]: 322.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Cheméo Relay (1.0)
logp	3.913		Crippen Method
mcvol	244.860	ml/mol	McGowan Method
tf	392.95	K	Cheméo Relay (1.0)

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U119670&Units=SI>
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
tf: Normal melting (fusion) point

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