(5R,6S,8S,Z)-8-Methoxy-3,6,10-trimethyl-4-oxo-4,5 acetate

Inchi:	InChI=1S/C18H24O5/c1-10-6-14(21-5)8-11(2)18(23-13(4)19)17(20)16-12(3)9-22-15(16)7
InchiKey:	DCFSJMWNJKXQCQ-POHAHGRESA-N
Formula:	C18H24O5
SMILES:	COC1C=C(C)Cc2occ(C)c2C(=O)C(OC(C)=O)C(C)C1
Mol. weight [g/mol]:	320.38
CAS:	383368-25-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.59		Crippen Method
logp	3.246		Crippen Method
mcvol	250.610	ml/mol	McGowan Method
rinpol	2065.70		NIST Webbook
rinpol	2065.70		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C383368250&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

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