Sceleratine

Inchi:	InChI=1S/C18H27NO7/c1-10-11(2)18(24,9-20)16(22)26-13-5-7-19-6-4-12(14(13)19)8-25
InchiKey:	KWEQCWXCFQWUQU-QGROXRHPSA-N
Formula:	C18H27NO7
SMILES:	CC1C(C)C(O)(CO)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23
Mol. weight [g/mol]:	369.41
CAS:	6190-25-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Crippen Method
logp	-0.784		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
rinpol	2545.00		NIST Webbook
rinpol	2546.00		NIST Webbook

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=C6190256&Units=SI

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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https://www.chemeo.com/cid/50-292-2/Sceleratine.pdf

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