Grahamine

Inchi:	InChI=1S/C21H31NO7/c1-6-12(2)17(23)29-21(5)13(3)18(24)28-15-8-10-22-9-7-14(16(15
InchiKey:	BGODDTSFBHJRGK-UHFFFAOYSA-N
Formula:	C21H31NO7
SMILES:	CCC(C)C(=O)OC1(C)C(C)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23
Mol. weight [g/mol]:	409.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	1.204		Crippen Method
mcvol	308.040	ml/mol	McGowan Method
rinpol	2711.00		NIST Webbook
rinpol	2711.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R590297&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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