1-Naphthalenecarboxylic acid, 5-[2-(3-furanyl)ethyl]-3,4,4a,5,6,7,8,8a-octahydro-5 methyl ester, [4aS-(4a«alpha»,5«alpha»,6«beta»,8a«beta»)]-

Other names:	Methyl (+)-hardwickiate
Inchi:	InChI=1S/C21H30O3/c1-15-8-11-21(3)17(19(22)23-4)6-5-7-18(21)20(15,2)12-9-16-10-13
InchiKey:	[illegible]
Formula:	C21H30O3
SMILES:	COC(=O)C1=CCCC2C1(C)CCC(C)C2(C)CCc1ccoc1
Mol. weight [g/mol]:	330.46
CAS:	56630-98-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.83		Crippen Method
logp	5.164		Crippen Method
mcvol	274.580	ml/mol	McGowan Method
rinpol	2455.20		NIST Webbook
rinpol	2455.20		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56630989&Units=SI
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

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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