

Heptadecan-1-ol, nicotinate

Other names:	Nicotinic acid, heptadecyl ester
Inchi:	InChI=1S/C23H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-26-23(25)22-18-17-
InchiKey:	NBHWTRRFTRBYCL-UHFFFAOYSA-N
Formula:	C23H39NO2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]:	361.56
CAS:	862594-96-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.18		Crippen Method
logp	7.110		Crippen Method
mcvol	328.590	ml/mol	McGowan Method
rinpol	2752.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C862594965&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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<https://www.chemeo.com/cid/30-409-4/Heptadecan-1-ol-nicotinate.pdf>

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