

Nicotinic acid, propyl ester

Other names:	propyl nicotinate
Inchi:	InChI=1S/C9H11NO2/c1-2-6-12-9(11)8-4-3-5-10-7-8/h3-5,7H,2,6H2,1H3
InchiKey:	CLAOCVWIKGTOP-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCCOC(=O)c1cccnc1
Mol. weight [g/mol]:	165.19
CAS:	7681-15-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	1.648		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
rinpola	1294.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7681154&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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