

4-Pyridinecarboxylic acid, butyl ester

Other names:	Butyl isonicotinate Isonicotinic acid, butyl ester NSC 83155
Inchi:	InChI=1S/C10H13NO2/c1-2-3-8-13-10(12)9-4-6-11-7-5-9/h4-7H,2-3,8H2,1H3
InchiKey:	UMQFMEMKBWWILL-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCCOC(=O)c1ccncc1
Mol. weight [g/mol]:	179.22
CAS:	13841-66-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	2.038		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13841662&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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