

Butyl nicotinate

Other names:	3-Pyridinecarboxylic acid, butyl ester Ba 2674 Butyl 3-pyridinecarboxylate Nicotinic acid butyl ester Nicotinic acid n-butyl ester butyl pyridine-3-carboxylate n-Butyl nicotinate
Inchi:	InChI=1S/C10H13NO2/c1-2-3-7-13-10(12)9-5-4-6-11-8-9/h4-6,8H,2-3,7H2,1H3
InchiKey:	DQULIMIQTCDUAN-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCCOC(=O)c1cccnc1
Mol. weight [g/mol]:	179.22
CAS:	6938-06-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.84		Aqueous Solubility Prediction Method
logp	2.038		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6938063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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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