

2-(n-Propylthio)nicotinic acid

Inchi:	InChI=1S/C9H11NO2S/c1-2-6-13-8-7(9(11)12)4-3-5-10-8/h3-5H,2,6H2,1H3,(H,11,12)
InchiKey:	CSMDLVRDBYKTAH-UHFFFAOYSA-N
Formula:	C9H11NO2S
SMILES:	CCCS _{c1} ncccc1C(=O)O
Mol. weight [g/mol]:	197.25
CAS:	175135-22-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	2.282		Crippen Method
mvol	147.680	ml/mol	McGowan Method

Sources

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=C175135225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

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