

2-Hydroxypyridine, pentafluoropropionate

Inchi:	InChI=1S/C8H4F5NO2/c9-7(10,8(11,12)13)6(15)16-5-3-1-2-4-14-5/h1-4H
InchiKey:	WHSGEUAHAXMJCQ-UHFFFAOYSA-N
Formula:	C8H4F5NO2
SMILES:	O=C(Oc1ccccn1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	241.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	2.185		Crippen Method
mcvol	126.090	ml/mol	McGowan Method
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376216&Units=SI
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

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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