

3-Hydroxypyridine, heptafluorobutyrate

Inchi:	InChI=1S/C9H4F7NO2/c10-7(11,8(12,13)9(14,15)16)6(18)19-5-2-1-3-17-4-5/h1-4H
InchiKey:	XDJQZXYPLKZVNL-UHFFFAOYSA-N
Formula:	C9H4F7NO2
SMILES:	O=C(Oc1cccnc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	291.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.820		Crippen Method
mcvol	143.720	ml/mol	McGowan Method
rinpole	965.00		NIST Webbook
rinpole	965.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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