

4H-3,1-Benzoxazine-4-one, 2-heptafluoropropyl-

Inchi:	InChI=1S/C11H4F7NO2/c12-9(13,10(14,15)11(16,17)18)8-19-6-4-2-1-3-5(6)7(20)21-8/h
InchiKey:	LEJAJVFLTGIPPE-UHFFFAOYSA-N
Formula:	C11H4F7NO2
SMILES:	O=c1oc(C(F)(F)C(F)(F)C(F)(F)F)nc2ccccc12
Mol. weight [g/mol]:	315.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	3.477		Crippen Method
mcvol	156.740	ml/mol	McGowan Method
rinpol	1266.00		NIST Webbook
rinpol	1266.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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