

1-Phenyl-2-pyrazyl-tetrafluoroethane

Inchi:	InChI=1S/C12H8F4N2/c13-11(14,9-4-2-1-3-5-9)12(15,16)10-8-17-6-7-18-10/h1-8H
InchiKey:	VOHULKRTQBHUJI-UHFFFAOYSA-N
Formula:	C12H8F4N2
SMILES:	FC(F)(c1ccccc1)C(F)(F)c1cnccn1
Mol. weight [g/mol]:	256.20
CAS:	116403-10-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.360		Crippen Method
mcvol	159.460	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=C116403102&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
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/117-906-6/1-Phenyl-2-pyrazyl-tetrafluoroethane.pdf>

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