

I-Proline, n-heptafluorobutyryl-, isobutyl ester

Other names:	Proline, isobutyl ester, HFB
Inchi:	InChI=1S/C13H16F7NO3/c1-7(2)6-24-9(22)8-4-3-5-21(8)10(23)11(14,15)12(16,17)13(18)
InchiKey:	CUIFOXVDOLQLQM-UHFFFAOYSA-N
Formula:	C13H16F7NO3
SMILES:	CC(C)COC(=O)C1CCCN1C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	367.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	3.010		Crippen Method
mcvol	214.550	ml/mol	McGowan Method
rinpol	1468.00		NIST Webbook
rinpol	1468.00		NIST Webbook

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=U321098&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
rinpol:	Non-polar retention indices

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