

Alpha,alpha-difluorophenacyl pyrazine

Inchi:	InChI=1S/C12H8F2N2O/c13-12(14,10-8-15-6-7-16-10)11(17)9-4-2-1-3-5-9/h1-8H
InchiKey:	HFQPREQQACYNB-UHFFFAOYSA-N
Formula:	C12H8F2N2O
SMILES:	O=C(c1ccccc1)C(F)(F)c1cnccn1
Mol. weight [g/mol]:	234.20
CAS:	116403-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.65		Crippen Method
logp	2.451		Crippen Method
mcvol	157.490	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C116403022&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/27-940-8/Alpha-alpha-difluorophenacyl-pyrazine.pdf>

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