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: HFQPREQQQACYNB-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