2-Phenoxy-3-(alpha,alpha-difluorobenzyl) pyrazine

Inchi: InChI=1S/C17H12F2N2O/c18-17(19,13-7-3-1-4-8-13)15-16(21-12-11-20-15)22-14-9-5-2-
InchiKey: FTWUKTBCOJEGPG-UHFFFAOYSA-N
Formula: C17H12F2N2O
SMILES: FC(F)(c1ccccc1)c1nccnc1Oc1ccccc1
Mol. weight [g/mol]: 298.29
CAS: 116403-01-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.11		Crippen Method
logp	4.409		Crippen Method
mcvol	208.480	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116403011&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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