Piperazine, 2-keto-1-(3-trifluoromethylphenyl), 4-acetyl, acetoxy-M

Inchi: InChI=1S/C15H15F3N2O4/c1-9(21)19-5-6-20(14(23)8-19)11-3-4-13(24-10(2)22)12(7-11)

InchiKey: ZLJDNCBIQATRNB-UHFFFAOYSA-N

Formula: C15H15F3N2O4

SMILES: CC(=O)Oc1ccc(N2CCN(C(C)=O)CC2=O)cc1C(F)(F)F

Mol. weight [g/mol]: 344.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.826		Crippen Method
mcvol	223.440	ml/mol	McGowan Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R404403&Units=SI

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

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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