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

Inchi: InChI=1S/C15H17F3N2O3/c1-10(21)19-5-7-20(8-6-19)12-3-4-14(23-11(2)22)13(9-12)15(

InchiKey: ZXAJSDPKUCRVQW-UHFFFAOYSA-N

Formula: C15H17F3N2O3

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

Mol. weight [g/mol]: 330.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Crippen Method
logp	2.299		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook

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=R404389&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.