1-(m-Trifluoromethylphenyl)piperazine, 4-trifluoroacetyl-

Other names: 1-(3-trifluoromethylphenyl)piperazine, TFA
Inchi: InChI=1S/C13H12F6N2O/c14-12(15,16)9-2-1-3-10(8-9)20-4-6-21(7-5-20)11(22)13(17,18
InchiKey: FEYWFZXNGXBSSF-UHFFFAOYSA-N
Formula: C13H12F6N2O
SMILES: O=C(N1CCN(c2cccc(C(F)(F)F)c2)CC1)C(F)(F)F
Mol. weight [g/mol]: 326.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	2.916		Crippen Method
mcvol	191.560	ml/mol	McGowan Method
rinpol	1724.00		NIST Webbook

Sources

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=U292946&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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