

Trifluoperidol

Other names:

Butyrophenone,
4'-fluoro-4-(4-hydroxy-4-(«alpha», «alpha», «alpha»-trifluoro-m-tolyl)piperidino)-
Flumoperone
McN-JR-2498
Psicoperidol
Psicoperidol-R
Psychoperidol
R-2498
Triperidol
Trisedil
Trisedyl
1-Butanone,
1-(4-fluorophenyl)-4-(4-hydroxy-4-(3-(trifluoromethyl)phenyl)-1-piperidinyl)-
4-Fluoro-4-(4-hydroxy-4-(«alpha», «alpha», «alpha»-trifluoro-m-tolyl)piperidino)butyrophenone
4-Fluoro-4,4-idrossi-4-(m-trifluorometil-fenil)-piperidino-butirrofenone
Trifluoperidolo
NSC 170978
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Inchi: InChI=1S/C22H23F4NO2/c23-19-8-6-16(7-9-19)20(28)5-2-12-27-13-10-21(29,11-14-27)**InchiKey:** GPMXUUPHFNMDH-UHFFFAOYSA-N**Formula:** C22H23F4NO2**SMILES:** O=C(CCCN1CCC(O)(c2cccc(C(F)(F)F)c2)CC1)c1ccc(F)cc1**Mol. weight [g/mol]:** 409.42**CAS:** 749-13-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	4.791		Crippen Method
mcvol	286.960	ml/mol	McGowan Method
rinpol	2645.00		NIST Webbook
rinpol	2665.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2665.00		NIST Webbook
rinpol	2645.00		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=C749133&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
rinpola:	Non-polar retention indices

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