Methylphenidate, N-trifluoroacetyl-

Other names:	Methyl phenyl[1-(trifluoroacetyl)-2-piperidinyl]acetate
	Methylphenidate, N-TFA
Inchi:	InChI=1S/C16H18F3NO3/c1-23-14(21)13(11-7-3-2-4-8-11)12-9-5-6-10-20(12)15(22)16(1
InchiKey:	VWHAIRLERWBGPH-UHFFFAOYSA-N
Formula:	C16H18F3NO3
SMILES:	COC(=O)C(c1ccccc1)C1CCCCN1C(=O)C(F)(F)F
Mol. weight [g/mol]:	329.31
CAS:	27765-90-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.887		Crippen Method
mcvol	225.980	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=C27765908&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

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