

Carbostyryl, n-methyl-6-(trifluoromethyl)-

Inchi:	InChI=1S/C11H8F3NO/c1-15-9-4-3-8(11(12,13)14)6-7(9)2-5-10(15)16/h2-6H,1H3
InchiKey:	BSFJLMNFTBGXQE-UHFFFAOYSA-N
Formula:	C11H8F3NO
SMILES:	Cn1c(=O)ccc2cc(C(F)(F)F)ccc21
Mol. weight [g/mol]:	227.18
CAS:	2261-94-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	2.557		Crippen Method
mcvol	143.790	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2261941&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/23-434-4/Carbostyryl-n-methyl-6-trifluoromethyl.pdf>

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