

Indoline, N-trifluoroacetyl-

Other names:	Indoline, TFA
Inchi:	InChI=1S/C10H8F3NO/c11-10(12,13)9(15)14-6-5-7-3-1-2-4-8(7)14/h1-4H,5-6H2
InchiKey:	NPSZSUAIVBOFOY-UHFFFAOYSA-N
Formula:	C10H8F3NO
SMILES:	O=C(N1CCc2ccccc21)C(F)(F)F
Mol. weight [g/mol]:	215.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	2.138		Crippen Method
mcvol	134.000	ml/mol	McGowan Method

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=U328352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/23-528-0/Indoline-N-trifluoroacetyl.pdf>

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