Purine, 6-(o-methoxyanilino)-

Inchi:	InChI=1S/C12H11N5O/c1-18-9-5-3-2-4-8(9)17-12-10-11(14-6-13-10)15-7-16-12/h2-7H,1
InchiKey:	IQOGGWLYHJXIIF-UHFFFAOYSA-N
Formula:	C12H11N5O
SMILES:	COc1ccccc1Nc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	241.25
CAS:	73663-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	1.623		Crippen Method
mcvol	173.030	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=C73663975&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

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