N-tert-Butyl-6-methoxy-1,3,5-triazine-2,4-diamine

Other names:	2-Amino-4-tert-butylamino-6-methoxy-1,3,5-triazine
	6-Methoxy-N-(2-methyl-2-propanyl)-1,3,5-triazine-2,4-diamine
	Deethylterbumeton
Inchi:	InChI=1S/C8H15N5O/c1-8(2,3)13-6-10-5(9)11-7(12-6)14-4/h1-4H3,(H3,9,10,11,12,13)
InchiKey:	HSYISQLUXXBNFW-UHFFFAOYSA-N
Formula:	C8H15N5O
SMILES:	COc1nc(N)nc(NC(C)(C)C)n1
Mol. weight [g/mol]:	197.24
CAS:	30125-64-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	0.673		Crippen Method
mcvol	155.590	ml/mol	McGowan Method
rinpol	1726.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30125645&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
rinpol:	Non-polar retention indices