

2-N-tert-butyl-4-N-ethyl-6-methoxy-1,3,5-triazine-2

Inchi:	InChI=1S/C10H19N5O/c1-6-11-7-12-8(15-10(2,3)4)14-9(13-7)16-5/h6H2,1-5H3,(H2,11,1
InchiKey:	BCQMBFHBZVHKU-UHFFFAOYSA-N
Formula:	C10H19N5O
SMILES:	CCNc1nc(NC(C)(C)C)nc(OC)n1
Mol. weight [g/mol]:	225.30

Physical Properties

Property code	Value	Unit	Source
hvap	97.64	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.59		Cheméo Relay (1.0)
logp	1.522		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
tf	399.53	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33693048&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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