Tropine

Other names:	Tropine
	1«alpha»H,5«alpha»H-Tropan-3«alpha»-ol
	Tropin
	2,3-Dihydro-3«alpha»-hydroxytropidine
	3«alpha»-Tropanol
	endo-8-Azabicyclo[3.2.1]-3-octanol, 8-methyl-
	N-Tropine (trans)
	Tropanol
	8-Methyl-8-azabicyclo[3.2.1]octan-3-ol, endo-
	8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, (3-endo)-
	NSC 43870
	8-Azabicyclo[3.2.1]octanol, 8-methyl-
	8-Methyl-8-azabicyclo[3.2.1]octan-3-ol
Inchi:	InChI=1S/C8H15NO/c1-9-6-2-3-7(9)5-8(10)4-6/h6-8,10H,2-5H2,1H3
InchiKey:	CYHOMWAPJJPNMW-UHFFFAOYSA-N
Formula:	C8H15NO
SMILES:	CN1C2CCC1CC(O)C2
Mol. weight [g/mol]:	141.21

Physical Properties

Property code	Value	Unit	Source
ie	8.10 ± 0.15	eV	NIST Webbook
log10ws	0.08		Cheméo Relay (1.0)
logp	0.604		Crippen Method
mcvol	117.710	ml/mol	McGowan Method
rinpol	1955.10		NIST Webbook
rinpol	1219.30		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1226.30		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1183.00		NIST Webbook
tb	506.20	K	NIST Webbook
tb	502.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120296&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature