Pseudotropine

Other names: exo-8-methyl-8-azabicyclo[3.2.1]octan-3-ol
8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, exo-
Inchi: InChI=1S/C9H17NO/c1-9(11)5-7-3-4-8(6-9)10(7)2/h7-8,11H,3-6H2,1-2H3
InchiKey: CELYWWIEPXTVDS-UHFFFAOYSA-N
Formula: C8H15NO
SMILES: CN1C2CCC1CC(C)(O)C2
Mol. weight [g/mol]: 141.21
CAS: 135-97-7

Physical Properties

Property code	Value	Unit	Source
ie	7.90 ± 0.15	eV	NIST Webbook
log10ws	-1.55		Crippen Method
logp	0.994		Crippen Method
mcvol	131.800	ml/mol	McGowan Method
rinpol	1233.70		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1233.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C135977&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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