6-Hydroxytropinone

Other names:	8-Azabicyclo[3.2.1]octan-3-one, 6-hydroxy-8-methyl-, exo- 7-hydroxy-8-methylazabicyclo[3.2.1]octan-3-one 6«beta»-Hydroxytropan-3-one
Inchi:	InChI=1S/C8H13NO2/c1-9-5-2-6(10)4-7(9)8(11)3-5/h5,7-8,11H,2-4H2,1H3
InchiKey:	UOHSTKWPZWFYTF-UHFFFAOYSA-N
Formula:	C8H13NO2
SMILES:	CN1C2CC(=O)CC1C(O)C2
Mol. weight [g/mol]:	155.19
CAS:	5932-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.41		Crippen Method
logp	-0.217		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5932536&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices