Tropinone

Other names:	8-Azabicyclo[3.2.1]octan-3-one, 8-methyl- 1«alpha»H,5«alpha»H-Tropan-3-one Tropanon Tropanone Tropinon 3-Tropanone 3-Tropinone Tropionone 8-Methyl-8-azabicyclo[3.2.1]octan-3-one 1Ah,5ah-tropan-3-one N-Methyl-8-azabicyclo[3.2.1]octan-3-one NSC 118012 1alphaH,5alphaH-Tropan-3-one
Inchi:	InChI=1S/C8H13NO/c1-9-6-2-3-7(9)5-8(10)4-6/h6-7H,2-5H2,1H3
InchiKey:	QQXLDOJGLXJCSE-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	CN1C2CCC1CC(=O)C2
Mol. weight [g/mol]:	139.19
CAS:	532-24-1

Physical Properties

Property code	Value	Unit	Source
ie	8.64	eV	NIST Webbook
log10ws	-1.03		Crippen Method
logp	0.812		Crippen Method
mcvol	113.410	ml/mol	McGowan Method
rinpol	1150.00		NIST Webbook
rinpol	1201.80		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1201.80		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1153.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.20	K	3.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C532241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure