

Imidazole, tetrahydro-1,3-dimethyl-2-(isopropylidene)

Inchi:	InChI=1S/C8H16N2/c1-7(2)8-9(3)5-6-10(8)4/h5-6H2,1-4H3
InchiKey:	YOUHIBLTNHWTPPL-UHFFFAOYSA-N
Formula:	C8H16N2
SMILES:	CC(C)=C1N(C)CCN1C
Mol. weight [g/mol]:	140.23
CAS:	109153-24-4

Physical Properties

Property code	Value	Unit	Source
ie	7.06	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.115		Crippen Method
mcvol	128.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109153244&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

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<https://www.chemeo.com/cid/15-037-4/Imidazole-tetrahydro-1-3-dimethyl-2-isopropylidene.pdf>

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