1,2-Benzisoxazole

Other names:	Indoxazene
	1-Oxa-2-azaindene
	1-Oxa-2-aza-1H-indene
	4,5-Benzisoxazole
	4,5-Benzisoazole
	benz[d]isoxazole
Inchi:	InChI=1S/C7H5NO/c1-2-4-7-6(3-1)5-8-9-7/h1-5H
InchiKey:	KTZQTRPPVKQPFO-UHFFFAOYSA-N
Formula:	C7H5NO
SMILES:	c1ccc2oncc2c1
Mol. weight [g/mol]:	119.12
CAS:	271-95-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.78		Crippen Method
logp	1.828		Crippen Method
mcvol	86.420	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.20	K	2.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C271954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure