

2,1-Benzisoxazole

Other names:	Anthranil benz[c]isoxazole
Inchi:	InChI=1S/C7H5NO/c1-2-4-7-6(3-1)5-9-8-7/h1-5H
InchiKey:	FZKCAHQKNJXICB-UHFFFAOYSA-N
Formula:	C7H5NO
SMILES:	c1ccc2nocc2c1
Mol. weight [g/mol]:	119.12
CAS:	271-58-9

Physical Properties

Property code	Value	Unit	Source
hvap	55.30 ± 0.30	kJ/mol	NIST Webbook
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	374.70	K	2.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C271589&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/53-053-4/2-1-Benzisoxazole.pdf>

Generated by Cheméo on 2024-05-01 22:12:30.294757065 +0000 UTC m=+16890799.215334381.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.