

Benzoselenazole

Other names: 1-Selena-3-azaindene
Inchi: InChI=1S/C7H5NSe/c1-2-4-7-6(3-1)8-5-9-7/h1-5H
InchiKey: AIGNCQCMONAWOL-UHFFFAOYSA-N
Formula: C7H5NSe
SMILES: c1ccc2[se]cnc2c1
Mol. weight [g/mol]: 182.08
CAS: 273-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.17		Crippen Method
logp	1.292		Crippen Method
tf	304.50 ± 0.50	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.00	K	2.70	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C273916&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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