

Benzo[b]selenophene

Other names:	Selenanaphthene Selenonaphthen Selenonaphthene
Inchi:	InChI=1S/C8H6Se/c1-2-4-8-7(3-1)5-6-9-8/h1-6H
InchiKey:	BNRDGHFESOHOBF-UHFFFAOYSA-N
Formula:	C8H6Se
SMILES:	c1ccc2[se]ccc2c1
Mol. weight [g/mol]:	181.09
CAS:	272-30-0

Physical Properties

Property code	Value	Unit	Source
ie	8.03 ± 0.05	eV	NIST Webbook
log10ws	-0.40		Crippen Method
logp	1.897		Crippen Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	512.30 ± 0.70	K	103.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C272300&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
tbrp:	Boiling point at reduced pressure

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