Benzeneselenol

Other names:	Benzene, selenyl-
	Phenol, seleno-
	Phenyl selenol
	Selenophenol
Inchi:	InChI=1S/C6H6Se/c7-6-4-2-1-3-5-6/h1-5,7H
InchiKey:	WDODWFPDZYSKIA-UHFFFAOYSA-N
Formula:	C6H6Se
SMILES:	[SeH]c1ccccc1
Mol. weight [g/mol]:	157.07
CAS:	645-96-5

Physical Properties

Property code	Value	Unit	Source
ie	7.70	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-2.73		Crippen Method
logp	0.213		Crippen Method
tb	456.70	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.40	kJ/mol	394.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.00 ± 1.00	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65661e+01
Coeff. B	-5.45713e+03
Temperature range (K), min.	331.00
Temperature range (K), max.	484.88

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645965&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure