1,2,3-Selenadiazole, 4-phenyl-

Inchi: InChI=1S/C8H6N2Se/c1-2-4-7(5-3-1)8-6-11-10-9-8/h1-6H
InchiKey: LEWDFWSHOZUNRZ-UHFFFAOYSA-N
Formula: C8H6N2Se
SMILES: c1ccc(-c2c[se]nn2)cc1
Mol. weight [g/mol]: 209.11
CAS: 25660-64-4

Physical Properties

Property code	Value	Unit	Source
chs	-4589.80 ± 8.40	kJ/mol	NIST Webbook
hf	452.30 ± 8.40	kJ/mol	NIST Webbook
hfs	358.00 ± 8.40	kJ/mol	NIST Webbook
hsub	94.10 ± 0.80	kJ/mol	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-0.73		Crippen Method
logp	1.201		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	90.70	kJ/mol	336.00	NIST Webbook
hsubt	91.20 ± 1.70	kJ/mol	309.00	NIST Webbook
hsubt	94.10 ± 0.80	kJ/mol	327.00	NIST Webbook

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=C25660644&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient