

Selenophene

Inchi: InChI=1S/C4H4Se/c1-2-4-5-3-1/h1-4H
InchiKey: MABNMNVCOAICNO-UHFFFAOYSA-N
Formula: C4H4Se
SMILES: c1cc[se]c1
Mol. weight [g/mol]: 131.03
CAS: 288-05-1

Physical Properties

Property code	Value	Unit	Source
hvap	38.10 ± 0.70	kJ/mol	NIST Webbook
ie	8.96	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
ie	9.01 ± 0.05	eV	NIST Webbook
ie	8.92	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.92	eV	NIST Webbook
ie	9.01 ± 0.05	eV	NIST Webbook
log10ws	1.40		Crippen Method
logp	0.744		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	47.10	kJ/mol	225.50	NIST Webbook
hvapt	40.80	kJ/mol	267.00	NIST Webbook
hvapt	34.00	kJ/mol	310.50	NIST Webbook

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.85069e+01
Coeff. B	-5.58093e+03
Coeff. C	1.82350e+01
Temperature range (K), min.	288.08
Temperature range (K), max.	404.71

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=C288051&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

hsubt:	Enthalpy of sublimation at a given temperature
hvac:	Enthalpy of vaporization at standard conditions
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

Latest version available from:

<https://www.chemeo.com/cid/63-729-3/Selenophene.pdf>

Generated by Cheméo on 2024-04-19 01:40:20.995431038 +0000 UTC m=+15780069.916008348.

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