

Carbon diselenide

Other names:	CSe2 Carbon selenide Carbon selenide (CSe2)
Inchi:	InChI=1S/CSe2/c2-1-3
InchiKey:	JNZSJDBNBJWXMZ-UHFFFAOYSA-N
Formula:	CSe2
SMILES:	[Se]=C=[Se]
Mol. weight [g/mol]:	169.93
CAS:	506-80-9

Physical Properties

Property code	Value	Unit	Source
affp	725.00	kJ/mol	NIST Webbook
basg	700.90	kJ/mol	NIST Webbook
ie	9.26 ± 0.00	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.40 ± 0.50	eV	NIST Webbook
ie	9.54 ± 0.01	eV	NIST Webbook
ie	9.27 ± 0.01	eV	NIST Webbook
ie	9.26 ± 0.01	eV	NIST Webbook
log10ws	4.96		Crippen Method
logp	-1.040		Crippen Method
sl	165.30	J/mol×K	NIST Webbook
tf	229.50 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	88.70	J/mol×K	298.00	NIST Webbook
hfust	6.36	kJ/mol	229.50	NIST Webbook
hsubt	46.30	kJ/mol	223.50	NIST Webbook

hvapt	39.10	kJ/mol	260.00	NIST Webbook
hvapt	35.90	kJ/mol	313.50	NIST Webbook
hvapt	39.00	kJ/mol	298.00	NIST Webbook
sfust	27.70	J/mol×K	229.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36802e+01
Coeff. B	-3.14206e+03
Coeff. C	-5.19150e+01
Temperature range (K), min.	286.53
Temperature range (K), max.	427.37

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=C506809&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
cpl:	Liquid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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

sfust: Entropy of fusion at a given temperature
sl: Liquid phase molar entropy at standard conditions
tf: Normal melting (fusion) point

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