1,10-Phenanthroline

Other names:	1,10-Fenanthrolin
	1,10-o-Phenanthroline
	4,5-diazaphenanthrene
	Activ-8 in hexylene glycol
	Orthophenanthroline
	Phenanthroline
	Solution forms containing 1,10-phenanthroline
	o-phenanthroline
	«beta»-Phenanthroline
Inchi:	InChI=1S/C12H8N2/c1-3-9-5-6-10-4-2-8-14-12(10)11(9)13-7-1/h1-8H
InchiKey:	DGEZNRSVGBDHLK-UHFFFAOYSA-N
Formula:	C12H8N2
SMILES:	c1cnc2c(c1)ccc1cccnc12
Mol. weight [g/mol]:	180.21

Physical Properties

Property code	Value	Unit	Source
af	0.4678		Cheméo Relay (1.0)
basg	908.00	kJ/mol	NIST Webbook
hf	310.16	kJ/mol	Cheméo Relay (1.0)
hfus	11.80	kJ/mol	Heat capacities and molar enthalpies and entropies of fusion for anhydrous 1,10-phenanthroline and 2,9-dimethyl-1,10-phenanthroline
hfus	15.50	kJ/mol	Thermodynamic properties of three-ring aza-aromatics. 2. Experimental results for 1,10-phenanthroline, phenanthridine, and 7,8-benzoquinoline, and mutual validation of experiments and computational methods
hvap	80.61	kJ/mol	Cheméo Relay (1.0)
ie	8.51 ± 0.02	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-1.53		Aqueous Solubility Prediction Method
logp	2.783		Crippen Method
mcvol	137.220	ml/mol	McGowan Method

pc	4664.76	kPa	Cheméo Relay (1.0, beta)
tb	621.13	K	Cheméo Relay (1.0)
tc	919.25	K	Cheméo Relay (1.0)
tf	390.48	K	Aqueous Solubility Prediction Method
tt	390.90	K	Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques
vc	0.525	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	15.50	kJ/mol	391.70	NIST Webbook
hfust	11.80	kJ/mol	391.10	NIST Webbook
hvapt	86.10	kJ/mol	298.00	Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography
hvapt	77.70 ± 0.10	kJ/mol	520.00	NIST Webbook
hvapt	74.90 ± 0.20	kJ/mol	560.00	NIST Webbook
hvapt	72.10 ± 0.20	kJ/mol	600.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66717&Units=SI

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Thermodynamic properties of three-ring aza-aromatics. 2. Experimental results for 1,10-phenanthroline, phenanthridine, and 7,8-benzoquinoline, and mutual validation of experiments and computational methods: https://www.doi.org/10.1016/j.jct.2009.11.011

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques: https://www.doi.org/10.1016/j.tca.2016.05.001

Study of the Anomalous Thermochemical Behavior of 1,2-Diazines by Correlation-Gas Chromatography: https://www.doi.org/10.1021/je900702t

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Heat capacities and molar enthalpies and entropies of fusion for anhydrous 1,10-phenanthroline and 2,9-dimethyl-1,10-phenanthroline: https://www.doi.org/10.1016/j.tca.2007.10.001

Legend

af:	Acentric Factor
basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume