1,7-Phenanthroline

Other names:	1,5-diazaphenanthrene
	1,7-phenantroline
	4,10-phenanthroline
	m-phenanthroline
	pyrido[2,3-f]quinoline
Inchi:	InChI=1S/C12H8N2/c1-3-9-5-6-11-10(4-2-7-13-11)12(9)14-8-1/h1-8H
InchiKey:	OZKOMUDCMCEDTM-UHFFFAOYSA-N
Formula:	C12H8N2
SMILES:	c1cnc2c(c1)ccc1ncccc12
Mol. weight [g/mol]:	180.21
CAS:	230-46-6

Physical Properties

Property code	Value	Unit	Source
hfus	18.20	kJ/mol	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds
hvap	79.40 ± 4.70	kJ/mol	NIST Webbook
log10ws	-2.68		Aqueous Solubility Prediction Method
log10ws	-2.68		Estimated Solubility Method
logp	2.783		Crippen Method
mcvol	137.220	ml/mol	McGowan Method
tt	351.70	K	Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C230466&Units=SI
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
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds.	https://www.doi.org/10.1021/je900034d
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tt:	Triple Point Temperature