

4,7-Phenanthroline

Inchi:	InChI=1S/C12H8N2/c1-3-9-10-4-2-8-14-12(10)6-5-11(9)13-7-1/h1-8H
InchiKey:	DATYUTWESAKQQM-UHFFFAOYSA-N
Formula:	C12H8N2
SMILES:	c1cnc2ccc3ncccc3c2c1
Mol. weight [g/mol]:	180.21
CAS:	230-07-9

Physical Properties

Property code	Value	Unit	Source
hfus	21.80	kJ/mol	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds
hvap	80.80 ± 4.70	kJ/mol	NIST Webbook
ie	8.35 ± 0.02	eV	NIST Webbook
log10ws	-4.61		Crippen Method
logp	2.783		Crippen Method
mcvol	137.220	ml/mol	McGowan Method
tt	444.10	K	Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques

Sources

Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds:	https://www.doi.org/10.1021/je900034d
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C230079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

Legend

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

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