Cinnoline

Other names:	Benzo[c]pyridazine
	«alpha»-Phenodiazine
	1,2-Benzodiazine
	1,2-Diazanaphthalene
Inchi:	InChI=1S/C8H6N2/c1-2-4-8-7(3-1)5-6-9-10-8/h1-6H
InchiKey:	WCZVZNOTHYJIEI-UHFFFAOYSA-N
Formula:	C8H6N2
SMILES:	c1ccc2nnccc2c1
Mol. weight [g/mol]:	130.15
CAS:	253-66-7

Physical Properties

Property code	Value	Unit	Source
affp	936.30	kJ/mol	NIST Webbook
basg	904.40	kJ/mol	NIST Webbook
ea	0.72 ± 0.10	eV	NIST Webbook
ie	8.51	eV	NIST Webbook
ie	8.95 ± 0.01	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	1.630		Crippen Method
mcvol	100.320	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	0.04	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C253667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ea:	Electron affinity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure