

ACENAPHTHO[1,2-b]QUINOXALINE

Other names:	7,10-Diaza-8,9-benzoflotruranthene 7,10-Diaza-8,9-benzofluoranthene 7,12-Diazabenz(o,k)fluoranthene
Inchi:	InChI=1S/C18H10N2/c1-2-10-15-14(9-1)19-17-12-7-3-5-11-6-4-8-13(16(11)12)18(17)20-
InchiKey:	VRSLSEDOBUYIMM-UHFFFAOYSA-N
Formula:	C18H10N2
SMILES:	c1cc2c3c(cccc3c1)-c1nc3ccccc3nc1-2
Mol. weight [g/mol]:	254.29

Physical Properties

Property code	Value	Unit	Source
hf	439.98	kJ/mol	Cheméo Relay (1.0)
hvap	114.49	kJ/mol	Cheméo Relay (1.0)
ie	8.60 ± 0.10	eV	NIST Webbook
log10ws	-5.99		Cheméo Relay (1.0)
logp	4.430		Crippen Method
mcvol	187.140	ml/mol	McGowan Method
tb	723.89	K	Cheméo Relay (1.0)
tf	505.10	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C207114&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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