

5,12-Diazatetracene-6,11-dione

Other names:	Benzo[b]phenazine-6,11-dione
Inchi:	InChI=1S/C16H8N2O2/c19-15-9-5-1-2-6-10(9)16(20)14-13(15)17-11-7-3-4-8-12(11)18-1
InchiKey:	QDORCAFTCNTEPU-UHFFFAOYSA-N
Formula:	C16H8N2O2
SMILES:	O=C1c2cccc2C(=O)c2nc3cccc3nc21
Mol. weight [g/mol]:	260.25

Physical Properties

Property code	Value	Unit	Source
hf	97.17	kJ/mol	Cheméo Relay (1.0)
ie	8.75	eV	Cheméo Relay (1.0)
log10ws	-4.68		Cheméo Relay (1.0)
logp	2.405		Crippen Method
mcvol	181.560	ml/mol	McGowan Method
tb	692.43	K	Cheméo Relay (1.0)
tf	569.01	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97594666&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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