Nickel octaethylporphyrin

Other names:	Ni-OEP complex
	2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine nickel
Inchi:	InChI=1S/C36H44N4.Ni/c1-9-21-22(10-2)30-18-32-25(13-5)26(14-6)34(39-32)20-36-28(1
InchiKey:	DIGQQRGHPATISA-XTPDIVBZSA-N
Formula:	C36H44N4Ni
SMILES:	CCC1=C(CC)c2cc3[n-]c(cc4nc(cc5[n-]c(cc1n2)c(CC)c5CC)C(CC)=C4CC)c(CC)c3CC.[Ni
Mol. weight [g/mol]:	591.45
CAS:	24803-99-4

Physical Properties

Property code	Value	Unit	Source
ie	6.38 ± 0.03	eV	NIST Webbook
rinpol	5410.00		NIST Webbook
rinpol	5410.00		NIST Webbook
rinpol	5410.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24803994&Units=SI
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
rinpol:	Non-polar retention indices

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