4-Isothiocyanato-4'-nitrodiphenyl ether

Other names: Benzene, 1-isothiocyanato-4-(4-nitrophenoxy)-
p-(p-Nitrophenoxy)phenyl isothiocyanate
Lopatol
Inchi: InChI=1S/C13H8N2O3S/c16-15(17)11-3-7-13(8-4-11)18-12-5-1-10(2-6-12)14-9-19/h1-8H
InchiKey: SVMGVZLUIWGYPH-UHFFFAOYSA-N
Formula: C13H8N2O3S
SMILES: O=[N+]([O-])c1ccc(Oc2ccc(N=C=S)cc2)cc1
Mol. weight [g/mol]: 272.28

Physical Properties

Property code	Value	Unit	Source
hf	212.70	kJ/mol	Cheméo Relay (1.0)
ie	8.11	eV	Cheméo Relay (1.0)
log10ws	-5.44		Cheméo Relay (1.0)
logp	4.121		Crippen Method
mcvol	187.530	ml/mol	McGowan Method
tb	636.11	K	Cheméo Relay (1.0)
tf	406.55	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=C19881186&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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