

Nitroscanate

Other names: Benzene, 1-isothiocyanato-4-(4-nitrophenoxy)-
p-(p-Nitrophenoxy)phenyl isothiocyanate
Lopatul

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

CAS: 19881-18-6

Physical Properties

Property code	Value	Unit	Source
hf	279.56	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.121		Crippen Method
mvol	187.530	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	880.37	K	Joback Method
tc	1174.42	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19881186&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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