

2-[(o-nitrophenyl)azo]-p-cresol

Other names:	Phenol, 4-methyl-2-[(2-nitrophenyl)azo]-
Inchi:	InChI=1S/C13H11N3O3/c1-9-6-7-13(17)11(8-9)15-14-10-4-2-3-5-12(10)16(18)19/h2-8,1
InchiKey:	DRPPFIRCMBJCM-UHFFFAOYSA-N
Formula:	C13H11N3O3
SMILES:	<chem>Cc1ccc(O)c(N=Nc2ccccc2[N+](=O)[O-])c1</chem>
Mol. weight [g/mol]:	257.24
CAS:	1435-71-8

Physical Properties

Property code	Value	Unit	Source
chs	-6886.40 ± 6.00	kJ/mol	NIST Webbook
chs	-6886.40 ± 6.00	kJ/mol	NIST Webbook
hf	-2.38	kJ/mol	Joback Method
hfs	198.70 ± 6.10	kJ/mol	NIST Webbook
hfs	198.70 ± 6.10	kJ/mol	NIST Webbook
hvap	86.68	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.024		Crippen Method
mcvol	185.460	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	941.82	K	Joback Method
tc	1226.24	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=C1435718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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