

2,2'-((1,8-Dihydroxy-3,6-disulfo-2,7-naphthylene)bis(azobenzene)arsonic acid

Other names:	2,7-bis(2-azonaphenylazo)-1,8-dihydroxynaphthalene-3,6-disulphonic acid
Inchi:	InChI=1S/C22H18As2N4O14S2/c29-21-18-11(9-16(43(37,38)39)19(21)27-25-14-7-3-1-5
InchiKey:	UQHVTNUJRKELCE-NBHCHVEOSA-N
Formula:	C22H18As2N4O14S2
SMILES:	O=S(=O)(O)c1cc2cc(S(=O)(=O)O)c(N=Nc3ccccc3[As](=O)(O)O)c(O)c2c(O)c1N=Nc1ccc
Mol. weight [g/mol]:	776.37
CAS:	1668-00-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.79		Crippen Method
logp	0.697		Crippen Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1668004&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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