

3-Azulenenesulfonic acid, 1,4-dimethyl-7-isopropyl-, sodium salt, hydrate

InChI:	InChI=1S/C15H18O3S.Na.H2O/c1-9(2)12-6-5-10(3)15-13(8-12)11(4)7-14(15)19(16,17)1
InChIKey:	MBPDRKMZHLMXCP-UHFFFAOYSA-M
Formula:	C15H19NaO4S
SMILES:	<chem>Cc1cc(S(=O)(=O)[O-])c2c(C)ccc(C(C)C)cc1-2.O.[Na+]</chem>
Mol. weight [g/mol]:	318.36

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007342&Units=SI>

Latest version available from:

<https://www.cheméo.com/cid/69-256-2/3-Azulenenesulfonic-acid-1-4-dimethyl-7-isopropyl-sodium-salt-hydrate.pdf>

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