

Sodium benzene sulfonate hydrate

Inchi: InChI=1S/C6H6O3S.Na.H2O/c7-10(8,9)6-4-2-1-3-5-6;;/h1-5H,(H,7,8,9);;1H2/q;+1;/p-1
InchiKey: OETNSIFETJNLBD-UHFFFAOYSA-M
Formula: C₆H₇NaO₄S
SMILES: O.O=S(=O)([O-])c1ccccc1.[Na+]
Mol. weight [g/mol]: 198.17

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001251&Units=SI>

Latest version available from:

<https://www.cheméo.com/cid/77-842-2/Sodium-benzene-sulfonate-hydrate.pdf>

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