

Hexocyclium (tral)

Inchi: InChI=1S/C20H33N2O.CH4O4S/c1-22(2)15-13-21(14-16-22)17-20(23,18-9-5-3-6-10-18)
InchiKey: NSILVESQCSUIAJ-UHFFFAOYSA-M
Formula: C₂₁H₃₆N₂O₅S
SMILES: COS(=O)(=O)[O-].C[N+]1(C)CCN(CC(O)(c2ccccc2)C2CCCCC2)CC1
Mol. weight [g/mol]: 428.59

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005039&Units=SI&Mask=3FFF>

Latest version available from:

<https://www.cheméo.com/cid/123-603-5/Hexocyclium-tral.pdf>

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