

This is the water solubility prediction by WSKOWIN for a chemical with CAS NO 9004-82-4:

Water Sol: 187.3 mg/L

SMILES : [Na]OS(=O)(=O)OC=CC=CCCCCCCCCCCCC
CHEM : SODIUM LAURYL ETHER SULFATE
MOL FOR: C16 H29 O6 S1 Na1
MOL WT : 372.46

This SMILE notation is not related to Sodium laureth sulphate which has the CAS NO 9004-82-4. See the structure below.

----- WSKOW v1.41 Results -----

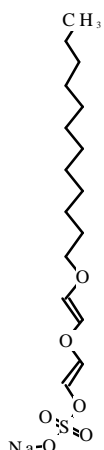
Log Kow (estimated) : 1.62
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 1.62

Equation Used to Make Water Sol estimate:

$\text{Log S (mol/L)} = 0.796 - 0.854 \log \text{Kow} - 0.00728 \text{ MW} + \text{Correction}$
(used when Melting Point NOT available)

Correction(s):	Value
-----	-----
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -3.299
Water Solubility at 25 deg C (mg/L): 187.3



Wat Sol (mg/L)(est): 187.3
SODIUM LAURYL ETHER SULFATE