

Benzofuran-2,3-dione, 2-[O-(2-hydroxyethyl)oxime], 3-(O-methyloxime), TMS, isomer 1

InChI: CC1=CC=C2C(=O)OC(=O)C2=C1O[Si](C)(C)C
InChIKey: TWWCBZQFCYXHFHK-UHFFFAOYSA-N

Formula: C₁₄H₂₀N₂O₄Si
SMILES: CON=C1C(=NOCCO[Si](C)(C)C)Oc2ccccc21
Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.60		Crippen Method
logp	2.611		Crippen Method
rinpol	2062.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook

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=R558842&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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