

Alpinon, TMS

Inchi: InChI=1S/C20H24O5Si/c1-22-14-11-15(23-2)17-16(12-14)24-19(13-9-7-6-8-10-13)20(18)
InchiKey: KLBKPHPOFFHLFX-UHFFFAOYSA-N
Formula: C20H24O5Si
SMILES: COc1cc(OC)c2c(c1)OC(c1cccc1)C(O[Si](C)(C)C)C2=O
Mol. weight [g/mol]: 372.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	4.240		Crippen Method
rinpol	2533.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R579567&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/58-963-9/Alpinon-TMS.pdf>

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