

GA88, MeTMS

Inchi: InChI=1S/C23H32O5Si/c1-13-11-22-12-14(13)7-8-15(22)23-10-9-16(28-29(4,5)6)21(2,20)
InchiKey: QSFNUIZPZNQETN-YAYLXUHMSA-N
Formula: C23H32O5Si
SMILES: C=C1CC23CC1CC=C2C12CCC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	4.004		Crippen Method
rinpol	2512.00		NIST Webbook
rinpol	2491.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2512.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R80059&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/50-480-3/GA88-MeTMS.pdf>

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