

GA126, MeTMS

Inchi: InChI=1S/C26H40O6Si2/c1-16-14-24-15-26(16,32-34(7,8)9)18(31-33(4,5)6)13-17(24)25-26
InchiKey: ADMBQZFCINCQTI-LFSDHFMUSA-N
Formula: C26H40O6Si2
SMILES: C=C1C[C@]23C[C@@]1(O[Si](C)(C)C)[C@@H](O[Si](C)(C)C)C[C@H]2[C@@]12C=CC1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4C5=CC=CC=C5C6=CC=CC=C6C7=CC=CC=C7C8=CC=CC=C8C9=CC=CC=C9C10=CC=CC=C10C11=CC=CC=C11C12=CC=CC=C12C13=CC=CC=C13C14=CC=CC=C14C15=CC=CC=C15C16=CC=CC=C16C17=CC=CC=C17C18=CC=CC=C18C19=CC=CC=C19C20=CC=CC=C20C21=CC=CC=C21C22=CC=CC=C22C23=CC=CC=C23C24=CC=CC=C24C25=CC=CC=C25C26=CC=CC=C26
Mol. weight [g/mol]: 504.77

Physical Properties

Property code	Value	Unit	Source
logp	4.834		Crippen Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R281200>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/124-490-0/GA126-MeTMS.pdf>

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