GA45, MeTMS

Inchi:	InChI=1S/C23H34O5Si/c1-13-14-8-9-15-22(12-14,18(13)28-29(4,5)6)16(19(24)26-3)17-2
InchiKey:	OUPGAIZPZYZAME-OEVRTZMNSA-N
Formula:	C23H34O5Si
SMILES:	C=C1C2CCC3C45CCCC(C)(C(=O)O4)C5C(C(=O)OC)C3(C2)C1O[Si](C)(C)C
Mol. weight [g/mol]:	418.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	4.084		Crippen Method
rinpol	2499.00		NIST Webbook
rinpol	2484.00		NIST Webbook
rinpol	2485.00		NIST Webbook
rinpol	2476.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R79583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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