

Alfaxalone, MO-TMS

Inchi:	InChI=1S/C26H46N2O3Si/c1-17(27-29-4)21-11-12-22-20-10-9-18-15-19(31-32(6,7)8)13-
InchiKey:	QNTUYUZHRGUGNY-DWHXGUJLSA-N
Formula:	C26H46N2O3Si
SMILES:	CON=C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(=NOC)CC12C
Mol. weight [g/mol]:	462.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	6.500		Crippen Method
rinpol	2880.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/37-057-8/Alfaxalone-MO-TMS.pdf>

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