

NIFLUMIC ACID TBDMS

Other names:	Niflumic acid, tbdms derivative
Inchi:	InChI=1S/C19H23F3N2O2Si/c1-18(2,3)27(4,5)26-17(25)15-10-7-11-23-16(15)24-14-9-6
InchiKey:	ABVMYTKMQZELRT-UHFFFAOYSA-N
Formula:	C19H23F3N2O2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1cccnc1Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	396.48

Physical Properties

Property code	Value	Unit	Source
hvap	91.56	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.73		Cheméo Relay (1.0)
logp	6.006		Crippen Method
rinpol	2335.60		NIST Webbook
rinpol	2335.60		NIST Webbook
tf	406.60	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U331798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/47-436-6/NIFLUMIC-ACID-TBDMS.pdf>

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