

1-Octadecanol, tert-butyldimethylsilyl ether

Other names:	1-Octadecanol, DMTBS 1-Octadecanol, O-TBDMS 1-Octadecanol, tBDMS 1-Octadecanol, tert-butyldimethylsilyl ether 1-Octadecyl tert-butyldimethylsilyl ether 1-Octadecanol, tbdms derivative
Inchi:	InChI=1S/C24H52OSi/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-26(5,6)2
InchiKey:	FLXIDOPWVJYZFM-UHFFFAOYSA-N
Formula:	C24H52OSi
SMILES:	CCCCCCCCCCCCCCCCCO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	384.76

Physical Properties

Property code	Value	Unit	Source
af	0.9502		Cheméo Relay (1.0)
hf	-759.48	kJ/mol	Cheméo Relay (1.0)
hvap	99.24	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
logp	9.270		Crippen Method
pc	695.67	kPa	Cheméo Relay (1.0, beta)
rinpol	2395.00		NIST Webbook
rinpol	2384.50		NIST Webbook
rinpol	2382.50		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	2384.50		NIST Webbook
rinpol	2395.00		NIST Webbook
ripol	2339.00		NIST Webbook
ripol	2339.00		NIST Webbook
ripol	2339.00		NIST Webbook
tb	606.21	K	Cheméo Relay (1.0)
tc	792.96	K	Cheméo Relay (1.0)
tf	280.07	K	Cheméo Relay (1.0)
vc	1.467	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C65598007&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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<https://www.chemeo.com/cid/95-510-0/1-Octadecanol-tert-butyldimethylsilyl-ether.pdf>

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