1-Trimethylsilyloxyoctadecane

Other names:	Octadecoxy-trimethylsilane
	1-(Trimethylsilyloxy)octadecane
	Octadecane, 1-trimethylsilyloxy-
	(Octadecyloxy)trimethylsilane
	1-Octadecanol, trimethylsilyl ether
	Octadecyl trimethylsilyl ether
	1-Octadecanol, O-TMS
	Octadecan-1-ol, TMS ether
	Trimethyl(octadecyloxy)silane
	1-Octadecanol, TMS
	1-Octadecanol, tms derivative
Inchi:	InChI=1S/C21H46OSi/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(2,3)4/h
InchiKey:	GVPDNFYOFKBFEN-UHFFFAOYSA-N
Formula:	C21H46OSi
SMILES:	CCCCCCCCCCCCCCCCCCO[Si](C)(C)C
Mol. weight [g/mol]:	342.68

Physical Properties

Property code	Value	Unit	Source
af	0.9129		Cheméo Relay (1.0)
gf	9.65	kJ/mol	Cheméo Relay (1.0, beta)
hf	-733.67	kJ/mol	Cheméo Relay (1.0)
hvap	96.19	kJ/mol	Cheméo Relay (1.0)
ie	9.90	eV	Cheméo Relay (1.0)
log10ws	-7.76		Cheméo Relay (1.0)
logp	8.099		Crippen Method
pc	610.88	kPa	Cheméo Relay (1.0, beta)
rinpol	2165.00		NIST Webbook
rinpol	2149.10		NIST Webbook
rinpol	2149.10		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2159.00		NIST Webbook

rinpol	2145.30		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2135.00		NIST Webbook
tb	594.79	K	Cheméo Relay (1.0)
tc	748.65	K	Cheméo Relay (1.0)
tf	282.83	K	Cheméo Relay (1.0)
vc	1.337	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18748986&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
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