

Heptan-1-ol, tert-butyldimethylsilyl ether

Inchi:	InChI=1S/C13H30OSi/c1-7-8-9-10-11-12-14-15(5,6)13(2,3)4/h7-12H2,1-6H3
InchiKey:	SSKLQKJXKUEL BH-UHFFFAOYSA-N
Formula:	C13H30OSi
SMILES:	CCCCCCCCO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	230.47

Physical Properties

Property code	Value	Unit	Source
af	0.5524		Cheméo Relay (1.0)
hf	-529.75	kJ/mol	Cheméo Relay (1.0)
hvap	53.78	kJ/mol	Cheméo Relay (1.0)
ie	9.27	eV	Cheméo Relay (1.0)
logp	4.979		Crippen Method
pc	1726.88	kPa	Cheméo Relay (1.0, beta)
rinpol	1293.40		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1293.40		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
tb	503.07	K	Cheméo Relay (1.0)
tc	676.73	K	Cheméo Relay (1.0)
tf	229.30	K	Cheméo Relay (1.0)
vc	0.836	m3/kmol	Cheméo Relay (1.0)

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C115306893&Units=SI>

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

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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