

Heptanoic acid, tert-butyldimethylsilyl ester

Other names:	Heptanoic acid, tert-butyldimethylsilyl ester tert-Butyl(dimethyl)silyl heptanoate Heptanoic acid, DMTBS Heptanoic acid, TBDMS Heptanoic acid, tbdms derivative
Inchi:	InChI=1S/C13H28O2Si/c1-7-8-9-10-11-12(14)15-16(5,6)13(2,3)4/h7-11H2,1-6H3
InchiKey:	RHWPBALXGUQVAC-UHFFFAOYSA-N
Formula:	C13H28O2Si
SMILES:	CCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	244.45

Physical Properties

Property code	Value	Unit	Source
hf	-723.62	kJ/mol	Cheméo Relay (1.0)
hvap	60.11	kJ/mol	Cheméo Relay (1.0)
ie	9.67	eV	Cheméo Relay (1.0)
log10ws	-3.80		Cheméo Relay (1.0)
logp	4.505		Crippen Method
pc	1685.91	kPa	Cheméo Relay (1.0, beta)
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1383.10		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1383.10		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook
tb	503.22	K	Cheméo Relay (1.0)
tc	694.24	K	Cheméo Relay (1.0)
tf	255.02	K	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=C54251637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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