3-Aminobenzoic acid, N-acetyl-, trimethylsilyl ester

Inchi: InChI=1S/C12H17NO3Si/c1-9(14)13-11-7-5-6-10(8-11)12(15)16-17(2,3)4/h5-8H,1-4H3,(H

InchiKey: OKBYTWHKBWAONE-UHFFFAOYSA-N

Formula: C12H17NO3Si

SMILES: CC(=O)Nc1cccc(C(=O)O[Si](C)(C)C)c1

Mol. weight [g/mol]: 251.36

Physical Properties

Property code	Value	Unit	Source
hf	-637.34	kJ/mol	Cheméo Relay (1.0)
hvap	80.47	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-2.59		Cheméo Relay (1.0)
logp	2.637		Crippen Method
pc	1946.06	kPa	Cheméo Relay (1.0, beta)
rinpol	1958.00		NIST Webbook
rinpol	1958.00		NIST Webbook
tb	584.24	K	Cheméo Relay (1.0)
tc	809.39	K	Cheméo Relay (1.0)
tf	344.93	K	Cheméo Relay (1.0)

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375111&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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