

L-2-Aminobutyric acid, trimethylsilyl ester

Other names:	Trimethylsilyl (2R)-2-aminobutanoate L-2-aminobutyric acid, tms derivative
Inchi:	InChI=1S/C7H17NO2Si/c1-5-6(8)7(9)10-11(2,3)4/h6H,5,8H2,1-4H3
InchiKey:	DPRFUZUDPNMXIO-UHFFFAOYSA-N
Formula:	C7H17NO2Si
SMILES:	CCC(N)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	175.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Cheméo Relay (1.0)
logp	1.102		Crippen Method
rinpol	1031.50		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1031.50		NIST Webbook
rinpol	1047.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U332990&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/116-175-9/L-2-Aminobutyric-acid-trimethylsilyl-ester.pdf>

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