

Selenomethionine, N-(dimethylamino)methylene, O-butyl

Other names: (S,E)-Butyl 2-((dimethylamino)methyleneamino)-4-(methylselenanyl)butanoate
Inchi: InChI=1S/C12H24N2O2Se/c1-5-6-8-16-12(15)11(7-9-17-4)13-10-14(2)3/h10-11H,5-9H2
InchiKey: OHOLXAYVSBJS LF-UHFFFAOYSA-N
Formula: C12H24N2O2Se
SMILES: CCCCOC(=O)C(CC[Se]C)N=CN(C)C
Mol. weight [g/mol]: 307.29

Physical Properties

Property code	Value	Unit	Source
log10ws	0.41		Crippen Method
logp	1.849		Crippen Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U378744&Units=SI>

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/121-820-6/Selenomethionine-N-dimethylamino-methylene-O-butyl.pdf>

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