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

Other names: (S,E)-Methyl 2-((dimethylamino)methyleneamino)-4-(methylselanyl)butanoate
Inchi: InChI=1S/C9H18N2O2Se/c1-11(2)7-10-8(5-6-14-4)9(12)13-3/h7-8H,5-6H2,1-4H3
InchiKey: LHNCPTWZPDGBRC-UHFFFAOYSA-N
Formula: C9H18N2O2Se
SMILES: COC(=O)C(CC[Se]C)N=CN(C)C
Mol. weight [g/mol]: 265.21

Physical Properties

Property code	Value	Unit	Source
log10ws	1.67		Crippen Method
logp	0.679		Crippen Method
rinpol	1711.00		NIST Webbook
rinpol	1711.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U378746&Units=SI

Legend

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