

2,4,6,8,9,10-Hexaoxa-1,3,5,7-tetraarsatricyclo[3.3.1

Other names: 2,4,6,7,8,10-Hexaoxa-1,3,5,7-tetraarsatricyclo[3.3.1.1
Inchi: InChI=1S/As4O6/c5-1-6-3-8-2(5)9-4(7-1)10-3
InchiKey: KTTMEOWBIWLMSE-UHFFFAOYSA-N
Formula: As4O6
SMILES: O1[As]2O[As]3O[As]1O[As](O2)O3
Mol. weight [g/mol]: 395.68
CAS: 12505-67-8

Physical Properties

Property code	Value	Unit	Source
ie	10.30 ± 0.30	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
ie	10.01 ± 0.05	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
log10ws	8.97		Crippen Method
logp	-1.934		Crippen Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C12505678&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/86-136-6/2-4-6-8-9-10-Hexaoxa-1-3-5-7-tetraarsatricyclo-3-3-1-13-7-decane.pdf>

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