

Alpha-toluenearsonic acid

Inchi: InChI=1S/C7H9AsO3/c9-8(10,11)6-7-4-2-1-3-5-7/h1-5H,6H2,(H2,9,10,11)
InchiKey: ODQMOSYKHALMPU-UHFFFAOYSA-N
Formula: C7H9AsO3
SMILES: O=[As](O)(O)Cc1ccccc1
Mol. weight [g/mol]: 216.07
CAS: 620-27-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	0.122		Crippen Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C620279&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

Latest version available from:

<https://www.chemeo.com/cid/48-987-4/Alpha-toluenearsonic-acid.pdf>

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