

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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