Benzene, 1-azido-2-methyl-

Other names:	Toluene, o-azido-
	o-Azidotoluene
	o-Tolyl azide
Inchi:	InChI=1S/C7H7N3/c1-6-4-2-3-5-7(6)9-10-8/h2-5H,1H3
InchiKey:	ZKGVLNVASIPVAU-UHFFFAOYSA-N
Formula:	C7H7N3
SMILES:	Cc1ccccc1N=[N+]=[N-]
Mol. weight [g/mol]:	133.15
CAS:	31656-92-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.60		Crippen Method
logp	2.937		Crippen Method
mcvol	107.070	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.00 ± 1.00	K	1.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31656925&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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