

Benzene, 1-azido-3-methyl-

Other names:	Toluene, m-azido- m-Azidotoluene m-Tolyl azide 1-Azido-3-methylbenzene 3-Methylphenyl azide
Inchi:	InChI=1S/C7H7N3/c1-6-3-2-4-7(5-6)9-10-8/h2-5H,1H3
InchiKey:	WRMGCIOUNQGMSR-UHFFFAOYSA-N
Formula:	C7H7N3
SMILES:	<chem>Cc1cccc(N=[N+]=[N-])c1</chem>
Mol. weight [g/mol]:	133.15
CAS:	4113-72-8

Physical Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.50 ± 1.50	K	1.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4113728&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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