Benzene, azido-

Other names:	Azidobenzene
	Benzene, triazo-
	Phenyl azide
Inchi:	InChI=1S/C6H5N3/c7-9-8-6-4-2-1-3-5-6/h1-5H
InchiKey:	CTRLRINCMYICJO-UHFFFAOYSA-N
Formula:	C6H5N3
SMILES:	[N-]=[N+]=Nc1ccccc1
Mol. weight [g/mol]:	119.12
CAS:	622-37-7

Physical Properties

Property code	Value	Unit	Source
affp	820.00	kJ/mol	NIST Webbook
basg	787.50	kJ/mol	NIST Webbook
chl	-3420.00	kJ/mol	NIST Webbook
hvap	44.80 ± 0.80	kJ/mol	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.72 ± 0.02	eV	NIST Webbook
log10ws	-7.13		Crippen Method
logp	2.628		Crippen Method
mcvol	92.980	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.20	kJ/mol	358.00	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=C622377&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume