Benzene, 1-azido-4-nitro-

Other names:	1-Azido-4-nitrobenzen
	1-azido-4-nitrobenzene
	4-Nitrophenyl azide
	p-Azidonitrobenzene
	p-Nitrophenyl azide
Inchi:	InChI=1S/C6H4N4O2/c7-9-8-5-1-3-6(4-2-5)10(11)12/h1-4H
InchiKey:	CZZVSJPFJBUBDK-UHFFFAOYSA-N
Formula:	C6H4N4O2
SMILES:	[N-]=[N+]=Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	164.12
CAS:	1516-60-5

Physical Properties

Property code	Value	Unit	Source
chs	-3241.40 ± 4.20	kJ/mol	NIST Webbook
hf	389.70 ± 5.20	kJ/mol	NIST Webbook
hfs	308.70 ± 4.30	kJ/mol	NIST Webbook
hsub	81.00 ± 3.00	kJ/mol	NIST Webbook
log10ws	-7.78		Crippen Method
logp	2.537		Crippen Method
mcvol	110.400	ml/mol	McGowan Method
tf	341.40	K	Thermochemistry of organic azides revisited

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.10	kJ/mol	345.40	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of organic azides revisited:	https://www.doi.org/10.1016/j.tca.2014.10.015
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1516605&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point