

Azoxybenzene

Other names:	Diazene, diphenyl-, 1-oxide Azobenzene, oxide Azoxybenzide Diphenyldiazene N-oxide Azossibenzene Azoxybenzeen Azoxybenzol Benzene, azoxydi- Fenazox Fentoxan Diazene, 1,2-diphenyl-, 1-oxide NSC 1796
Inchi:	InChI=1S/C12H10N2O/c15-14(12-9-5-2-6-10-12)13-11-7-3-1-4-8-11/h1-10H
InchiKey:	GAUZCKBSTZFWCT-UHFFFAOYSA-N
Formula:	C12H10N2O
SMILES:	[O-][N+](=Nc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	198.22
CAS:	495-48-7

Physical Properties

Property code	Value	Unit	Source
chs	-6394.70 ± 1.50	kJ/mol	NIST Webbook
chs	-6450.50	kJ/mol	NIST Webbook
chs	-6450.50	kJ/mol	NIST Webbook
hf	342.00 ± 2.40	kJ/mol	NIST Webbook
hfs	299.00	kJ/mol	NIST Webbook
hfs	299.00	kJ/mol	NIST Webbook
hfs	243.40 ± 2.20	kJ/mol	NIST Webbook
hsub	98.60 ± 0.90	kJ/mol	NIST Webbook
ie	8.35	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.55	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
log10ws	-3.40		Crippen Method
logp	3.612		Crippen Method
mvol	153.950	ml/mol	McGowan Method

rinp	1846.00		NIST Webbook
tf	307.75 ± 0.50	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C495487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
rinp:	Non-polar retention indices
tf:	Normal melting (fusion) point

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