Benzene, nitroso-

Other names: Nitrosobenzene
Inchi: InChI=1S/C6H5NO/c8-7-6-4-2-1-3-5-6/h1-5H
InchiKey: NLRKCXQQSUWLCH-UHFFFAOYSA-N
Formula: C6H5NO
SMILES: O=Nc1ccccc1
Mol. weight [g/mol]: 107.11
CAS: 586-96-9

Physical Properties

Property code	Value	Unit	Source
affp	854.30	kJ/mol	NIST Webbook
basg	823.60	kJ/mol	NIST Webbook
chs	-3105.00 ± 6.30	kJ/mol	NIST Webbook
hf	201.00 ± 4.20	kJ/mol	NIST Webbook
hsub	80.80	kJ/mol	NIST Webbook
hvap	40.32	kJ/mol	Joback Method
ie	8.90 ± 0.10	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.87	eV	NIST Webbook
log10ws	-2.23		Crippen Method
logp	2.085		Crippen Method
mcvol	83.190	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	426.76	K	Joback Method
tc	640.08	K	Joback Method
tf	339.65 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	85.10	kJ/mol	318.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C586969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point