1-Nitro-2-nitrosobenzene

Inchi: InChI=1S/C6H4N2O3/c9-7-5-3-1-2-4-6(5)8(10)11/h1-4H
InchiKey: NSGVPXKWKUZSAY-UHFFFAOYSA-N
Formula: C6H4N2O3
SMILES: O=Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 152.11
CAS: 612-29-3

Physical Properties

Property code	Value	Unit	Source
chs	-3038.70 ± 1.90	kJ/mol	NIST Webbook
hf	-121.06	kJ/mol	Joback Method
hfs	102.30	kJ/mol	NIST Webbook
hsub	54.00	kJ/mol	NIST Webbook
hvap	57.58	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.993		Crippen Method
mcvol	100.610	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	583.58	K	Joback Method
tc	830.33	K	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C612293&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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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