p-DINITROSOBENZENE

Other names: Benzene, 1,4-dinitroso-
Benzene, p-dinitroso-
1,4-Dinitrosobenzene
Inchi: InChI=1S/C6H4N2O2/c9-7-5-1-2-6(8-10)4-3-5/h1-4H
InchiKey: MKZXROSCOHNKDX-UHFFFAOYSA-N
Formula: C6H4N2O2
SMILES: O=Nc1ccc(N=O)cc1
Mol. weight [g/mol]: 136.11

Physical Properties

Property code	Value	Unit	Source
hf	223.90	kJ/mol	Cheméo Relay (1.0)
ie	9.28	eV	Cheméo Relay (1.0)
logp	2.482		Crippen Method
mcvol	94.740	ml/mol	McGowan Method
tf	468.08	K	Cheméo Relay (1.0)

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105124&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
ie: Ionization energy

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point