

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

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