

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
CAS:	105-12-4

Physical Properties

Property code	Value	Unit	Source
hf	-278.49	kJ/mol	Joback Method
hvap	50.08	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.482		Crippen Method
mcvol	94.740	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	495.14	K	Joback Method
tc	707.16	K	Joback Method

Sources

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=C105124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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