

Phenol, 4-(phenylazo)-

Other names:	4-(Phenylazo)phenol 4-Hydroxyazobenzene Atul Brilliant Oil Yellow G Brasilazina Oil Yellow O C.I. 11800 C.I. Solvent Yellow 7 NSC 3177 Organol Yellow AP Phenol, 4-(2-phenyldiazenyl)- Phenol, p-(phenylazo)- Pirocard Green 491 Solvent Yellow 7 Zlut rozpoustedlova 7 p-(Benzeneazo)phenol p-(Phenylazo)phenol p-Hydroxyazobenzene
Inchi:	InChI=1S/C12H10N2O/c15-12-8-6-11(7-9-12)14-13-10-4-2-1-3-5-10/h1-9,15H
InchiKey:	BEYOBVMPDRKTNR-UHFFFAOYSA-N
Formula:	C12H10N2O
SMILES:	Oc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]:	198.22
CAS:	1689-82-3

Physical Properties

Property code	Value	Unit	Source
chs	-6314.10	kJ/mol	NIST Webbook
hf	51.96	kJ/mol	Joback Method
hfs	163.00	kJ/mol	NIST Webbook
hvap	66.54	kJ/mol	Joback Method
log10ws	-3.94		Aqueous Solubility Prediction Method
logp	3.808		Crippen Method
mcvol	153.950	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	757.14	K	Joback Method
tc	1034.00	K	Joback Method

tf	427.65	K	Aqueous Solubility Prediction Method
tf	425.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.99	kJ/mol	425.20	NIST Webbook
hfust	32.99	kJ/mol	425.20	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1689823&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tf:	Normal melting (fusion) point

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