4-(M-nitrophenylazo)resorcinol

Inchi: InChI=1S/C12H9N3O4/c16-10-4-5-11(12(17)7-10)14-13-8-2-1-3-9(6-8)15(18)19/h1-7,16-
InchiKey: VXGDALQPLLWULX-YPKPFQOOSA-N
Formula: C12H9N3O4
SMILES: O=[N+]([O-])c1cccc(N=Nc2ccc(O)cc2O)c1
Mol. weight [g/mol]: 259.22
CAS: 2243-74-5

Physical Properties

Property code	Value	Unit	Source
hf	-147.58	kJ/mol	Joback Method
hvap	96.81	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.421		Crippen Method
mcvol	177.240	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	994.58	K	Joback Method
tc	1287.77	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2243745&Units=SI
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

Legend

hf: Enthalpy of formation 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