

Benzenamine, 4-(4-nitrophenyl)-

Other names:	4-Amino-4'-nitrobiphenyl 4'-Nitro-4-biphenylamine [1,1'-Biphenyl]-4-amine, 4'-nitro- Benzenamine, 4-(4-nitrophenyl)-
Inchi:	InChI=1S/C12H10N2O2/c13-11-5-1-9(2-6-11)10-3-7-12(8-4-10)14(15)16/h1-8H,13H2
InchiKey:	BOFVBIYTBGDQGY-UHFFFAOYSA-N
Formula:	C12H10N2O2
SMILES:	Nc1ccc(-c2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]:	214.22

Physical Properties

Property code	Value	Unit	Source
hf	155.27	kJ/mol	Cheméo Relay (1.0)
hfus	30.70	kJ/mol	Joback Method
hvap	106.73	kJ/mol	Cheméo Relay (1.0)
ie	7.46 ± 0.03	eV	NIST Webbook
log10ws	-4.00		Cheméo Relay (1.0)
logp	2.844		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
tb	655.70	K	Cheméo Relay (1.0)
tf	431.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.24	J/mol×K	761.65	Joback Method
cpg	438.56	J/mol×K	808.19	Joback Method
cpg	449.65	J/mol×K	854.74	Joback Method
cpg	459.62	J/mol×K	901.28	Joback Method
cpg	468.56	J/mol×K	947.82	Joback Method
cpg	476.58	J/mol×K	994.36	Joback Method
cpg	483.76	J/mol×K	1040.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1211401&Units=SI
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):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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