

Benzenamine, 4-nitro-N-phenyl-

Other names:	Diphenylamine, 4-nitro- p-Nitrodiphenylamine 4-Nitrodiphenylamine 4-Nitrodifenylamin p-Nitrophenylphenylamine 4-nitro-N-phenylaniline N-(4-nitrophenyl)-N-phenylamine
Inchi:	InChI=1S/C12H10N2O2/c15-14(16)12-8-6-11(7-9-12)13-10-4-2-1-3-5-10/h1-9,13H
InchiKey:	XXYMSQQCBUKFHE-UHFFFAOYSA-N
Formula:	C12H10N2O2
SMILES:	O=[N+](O-)[c1ccc(Nc2ccccc2)cc1]
Mol. weight [g/mol]:	214.22
CAS:	836-30-6

Physical Properties

Property code	Value	Unit	Source
gf	390.29	kJ/mol	Joback Method
hf	213.29	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	70.55	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.338		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	734.31	K	Joback Method
tc	1004.26	K	Joback Method
tf	486.63	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.30	J/mol×K	734.31	Joback Method
cpg	434.25	J/mol×K	779.30	Joback Method

cpg	445.95	J/mol×K	824.29	Joback Method
cpg	456.48	J/mol×K	869.29	Joback Method
cpg	465.95	J/mol×K	914.28	Joback Method
cpg	474.47	J/mol×K	959.27	Joback Method
cpg	482.14	J/mol×K	1004.26	Joback Method
hsubt	130.60	kJ/mol	392.50	NIST Webbook

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=C836306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation 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
vc:	Critical Volume

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