Phenol, 4-(4-nitrophenyl)amino-

Other names: 4'-hydroxy-4-nitrodiphenylamine
Inchi: InChI=1S/C12H10N2O3/c15-12-7-3-10(4-8-12)13-9-1-5-11(6-2-9)14(16)17/h1-8,13,15H
InchiKey: VFFBUUIATYUJSZ-UHFFFAOYSA-N
Formula: C12H10N2O3
SMILES: O=[N+]([O-])c1ccc(Nc2ccc(O)cc2)cc1
Mol. weight [g/mol]: 230.22
CAS: 16078-86-7

Physical Properties

Property code	Value	Unit	Source
gf	235.67	kJ/mol	Joback Method
hf	35.98	kJ/mol	Joback Method
hfus	36.77	kJ/mol	Joback Method
hvap	83.56	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.044		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
tb	814.93	K	Joback Method
tc	1089.62	K	Joback Method
tf	598.35	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.46	J/mol×K	814.93	Joback Method
cpg	473.65	J/mol×K	860.71	Joback Method
cpg	484.10	J/mol×K	906.49	Joback Method
cpg	493.97	J/mol×K	952.28	Joback Method
cpg	503.47	J/mol×K	998.06	Joback Method
cpg	512.78	J/mol×K	1043.84	Joback Method
cpg	522.07	J/mol×K	1089.62	Joback Method

Sources

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=C16078867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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