Aniline, 4-(4-nitrophenyl)amino-

Other names: N-(4-nitrophenyl)-1,4-Benzenediamine
Inchi: InChI=1S/C12H11N3O2/c13-9-1-3-10(4-2-9)14-11-5-7-12(8-6-11)15(16)17/h1-8,14H,13H
InchiKey: XHVFCOOFJKCIAP-UHFFFAOYSA-N
Formula: C12H11N3O2
SMILES: Nc1ccc(Nc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 229.23
CAS: 6149-34-4

Physical Properties

Property code	Value	Unit	Source
gf	447.11	kJ/mol	Joback Method
hf	235.61	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	81.85	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.921		Crippen Method
mcvol	169.800	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	811.82	K	Joback Method
tc	1085.24	K	Joback Method
tf	582.41	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.71	J/mol×K	811.82	Joback Method
cpg	485.27	J/mol×K	857.39	Joback Method
cpg	495.66	J/mol×K	902.96	Joback Method
cpg	504.99	J/mol×K	948.53	Joback Method
cpg	513.36	J/mol×K	994.10	Joback Method
cpg	520.86	J/mol×K	1039.67	Joback Method
cpg	527.60	J/mol×K	1085.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6149344&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

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