4-Amino-3-nitro biphenyl

Other names: 3-nitrobiphenyl-4-ylamine
Inchi: InChI=1S/C12H10N2O2/c13-11-7-6-10(8-12(11)14(15)16)9-4-2-1-3-5-9/h1-8H,13H2
InchiKey: MQDYZYVWFUIEQU-UHFFFAOYSA-N
Formula: C12H10N2O2
SMILES: Nc1ccc(-c2ccccc2)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 214.22
CAS: 4085-18-1

Physical Properties

Property code	Value	Unit	Source
gf	357.72	kJ/mol	Joback Method
hf	182.14	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	75.41	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	2.844		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	761.65	K	Joback Method
tc	1040.91	K	Joback Method
tf	529.75	K	Joback Method
vc	0.603	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4085181&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

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