4-(4-Nitrophenoxy)aniline

Other names: 4-(4-nitrophenoxy)aniline
Inchi: InChI=1S/C12H10N2O3/c13-9-1-5-11(6-2-9)17-12-7-3-10(4-8-12)14(15)16/h1-8H,13H2
InchiKey: ASAOLTVUTGZJST-UHFFFAOYSA-N
Formula: C12H10N2O3
SMILES: Nc1ccc(Oc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 230.22

Physical Properties

Property code	Value	Unit	Source
hf	25.27	kJ/mol	Cheméo Relay (1.0)
hfus	31.89	kJ/mol	Joback Method
hvap	102.96	kJ/mol	Cheméo Relay (1.0)
ie	7.59	eV	Cheméo Relay (1.0)
log10ws	-4.02		Cheméo Relay (1.0)
logp	2.969		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
tb	646.17	K	Cheméo Relay (1.0)
tf	426.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.11	J/mol×K	784.07	Joback Method
cpg	462.01	J/mol×K	829.69	Joback Method
cpg	472.67	J/mol×K	875.31	Joback Method
cpg	482.15	J/mol×K	920.93	Joback Method
cpg	490.52	J/mol×K	966.55	Joback Method
cpg	497.84	J/mol×K	1012.17	Joback Method
cpg	504.17	J/mol×K	1057.79	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6149333&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

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