4'-Nitrobenzanilide

Other names:	N-Benzoyl-p-nitroaniline
	p'-Nitrobenzanilide
	Benzamide, N-(4-nitrophenyl)-
	Aniline, N-benzoyl-p-nitro-
	Benzamide, N-(p-nitrophenyl)-
	Benzanilide, 4'-nitro-
	N-(p-Nitrophenyl)benzamide
	N-(4-Nitrophenyl)benzamide
	p-Nitro-N-benzoylaniline
	N-(4-Nitrophenyl)benzoic acid amide
Inchi:	InChI=1S/C13H10N2O3/c16-13(10-4-2-1-3-5-10)14-11-6-8-12(9-7-11)15(17)18/h1-9H,(H
InchiKey:	GMGQGZYFQSCZCW-UHFFFAOYSA-N
Formula:	C13H10N2O3
SMILES:	O=C(Nc1ccc([N+](=O)[O-])cc1)c1ccccc1
Mol. weight [g/mol]:	242.23
CAS:	3393-96-2

Physical Properties

Property code	Value	Unit	Source
gf	269.79	kJ/mol	Joback Method
hf	80.07	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	79.52	kJ/mol	Joback Method
ie	8.60 ± 0.10	eV	NIST Webbook
log10ws	-4.10		Crippen Method
logp	2.847		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	811.06	K	Joback Method
tc	1078.56	K	Joback Method
tf	547.83	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.46	J/mol×K	811.06	Joback Method
cpg	492.83	J/mol×K	855.64	Joback Method
cpg	503.02	J/mol×K	900.23	Joback Method
cpg	512.13	J/mol×K	944.81	Joback Method
cpg	520.26	J/mol×K	989.39	Joback Method
cpg	527.51	J/mol×K	1033.98	Joback Method
cpg	533.99	J/mol×K	1078.56	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3393962&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
ie: Ionization energy
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