Methanone, (2-amino-5-nitrophenyl)phenyl-

Other names:	2-Amino-5-nitrobenzophenone
	(2-Amino-5-nitrophenyl)phenylmethanone
	5-Nitro-2-aminobenzophenone
	Benzophenone, 2-amino-5-nitro-
Inchi:	InChI=1S/C13H10N2O3/c14-12-7-6-10(15(17)18)8-11(12)13(16)9-4-2-1-3-5-9/h1-8H,14H
InchiKey:	PZPZDEIASIKHPY-UHFFFAOYSA-N
Formula:	C13H10N2O3
SMILES:	Nc1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1
Mol. weight [g/mol]:	242.23
CAS:	1775-95-7

Physical Properties

Property code	Value	Unit	Source
gf	237.22	kJ/mol	Joback Method
hf	48.92	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.408		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	838.40	K	Joback Method
tc	1114.24	K	Joback Method
tf	590.95	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.11	J/mol×K	838.40	Joback Method
cpg	495.88	J/mol×K	884.37	Joback Method
cpg	505.51	J/mol×K	930.35	Joback Method
cpg	514.07	J/mol×K	976.32	Joback Method
cpg	521.67	J/mol×K	1022.29	Joback Method
cpg	528.41	J/mol×K	1068.26	Joback Method
cpg	534.39	J/mol×K	1114.24	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1775957&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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