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

Other names: 2-Amino-2'-chloro-5-nitrobenzophenone
2-Amino-5-nitro-2'-chlorbenzophenone
2-Amino-5-nitro-2'-chlorobenzophenone
Benzophenone, 2-amino-2'-chloro-5-nitro
Clonazepam, acid hydrolyzed

Inchi: InChI=1S/C13H9ClN2O3/c14-11-4-2-1-3-9(11)13(17)10-7-8(16(18)19)5-6-12(10)15/h1-7

InchiKey: GRDGBWVSVMLKBV-UHFFFAOYSA-N

Formula: C13H9ClN2O3

SMILES: Nc1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1Cl

Mol. weight [g/mol]: 276.68

CAS: 2011-66-7

Physical Properties

Property code	Value	Unit	Source
gf	215.66	kJ/mol	Joback Method
hf	21.71	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	89.43	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.061		Crippen Method
mcvol	187.720	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2516.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	880.81	K	Joback Method
tc	1158.06	K	Joback Method
tf	633.39	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.18	J/mol×K	880.81	Joback Method
cpg	510.60	J/mol×K	927.02	Joback Method
cpg	518.95	J/mol×K	973.23	Joback Method
cpg	526.32	J/mol×K	1019.44	Joback Method
cpg	532.80	J/mol×K	1065.64	Joback Method
cpg	538.49	J/mol×K	1111.85	Joback Method
cpg	543.47	J/mol×K	1158.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2011667&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