2-(2'-Amino-5'-bromobenzoyl)pyridine

Other names:	2-(2'-Amino-5'-bromobenzoyl)pyridine
	2-(2-Amino-5-brom-benzoyl)-pyridine
	2-(2-Amino-5-bromobenzoyl)-pyridine
	2-amino-5-bromobenzoylpyridine
	Bromazepam benzophenone
	Pyridine, 2-(2-amino-5-bromobenzoyl)
Inchi:	InChI=1S/C12H9BrN2O/c13-8-4-5-10(14)9(7-8)12(16)11-3-1-2-6-15-11/h1-7H,14H2
InchiKey:	KHVZPFKJBLTYCC-UHFFFAOYSA-N
Formula:	C12H9BrN2O
SMILES:	Nc1ccc(Br)cc1C(=O)c1ccccn1
Mol. weight [g/mol]:	277.12

Physical Properties

Property code	Value	Unit	Source
hvap	97.22	kJ/mol	Cheméo Relay (1.0)
ie	8.17	eV	Cheméo Relay (1.0)
log10ws	-3.57		Cheméo Relay (1.0)
logp	2.657		Crippen Method
mcvol	171.450	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	656.22	K	Cheméo Relay (1.0)
tf	408.67	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563560&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point