Benzoic acid, p-[[(dimethylamino)methylene]amino]-, methyl ester

Other names: 4-Aminobenzoic acid, N-dimethylaminomethylene-, methyl ester
Inchi: InChI=1S/C11H14N2O2/c1-13(2)8-12-10-6-4-9(5-7-10)11(14)15-3/h4-8H,1-3H3
InchiKey: NQVUPXYJLAGUBE-UHFFFAOYSA-N
Formula: C11H14N2O2
SMILES: COC(=O)c1ccc(N=CN(C)C)cc1
Mol. weight [g/mol]: 206.24
CAS: 29390-16-7

Physical Properties

Property code	Value	Unit	Source
hf	-140.36	kJ/mol	Joback Method
hvap	57.53	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.695		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	648.15	K	Joback Method
tc	870.46	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29390167&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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