4-Aminobenzoic acid, N-dimethylaminomethylene-, ethyl ester

Inchi: InChI=1S/C12H16N2O2/c1-4-16-12(15)10-5-7-11(8-6-10)13-9-14(2)3/h5-9H,4H2,1-3H3
InchiKey: GHHKNAGPUBEDLN-UHFFFAOYSA-N
Formula: C12H16N2O2
SMILES: CCOC(=O)c1ccc(N=CN(C)C)cc1
Mol. weight [g/mol]: 220.27

Physical Properties

Property code	Value	Unit	Source
hf	-161.00	kJ/mol	Joback Method
hvap	59.76	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.085		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tb	671.03	K	Joback Method
tc	889.48	K	Joback Method

Sources

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=U375816&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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