

P-phenylazo carbanilic acid, methyl ester

Inchi: InChI=1S/C14H13N3O2/c1-19-14(18)15-11-7-9-13(10-8-11)17-16-12-5-3-2-4-6-12/h2-10
InchiKey: ZGTUJVDJHBBQIQ-WUKNDPDISA-N
Formula: C14H13N3O2
SMILES: COC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 255.27
CAS: 92166-43-3

Physical Properties

Property code	Value	Unit	Source
hf	-14.81	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	4.280		Crippen Method
mcvol	193.680	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
tb	853.72	K	Joback Method
tc	1108.76	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C92166433&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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