P-phenylazo carbanilic acid,n-pentyl ester

Inchi: InChI=1S/C18H21N3O2/c1-2-3-7-14-23-18(22)19-15-10-12-17(13-11-15)21-20-16-8-5-4-
InchiKey: WNTMFCCTXKRZLX-QZQOTICOSA-N
Formula: C18H21N3O2
SMILES: CCCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 311.38
CAS: 93995-95-0

Physical Properties

Property code	Value	Unit	Source
hf	-97.37	kJ/mol	Joback Method
hvap	83.14	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.841		Crippen Method
mcvol	250.040	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
tb	945.24	K	Joback Method
tc	1186.02	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=C93995950&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature