P-phenylazo carbanilic acid, phenethyl ester

Inchi: InChI=1S/C21H19N3O2/c25-21(26-16-15-17-7-3-1-4-8-17)22-18-11-13-20(14-12-18)24-2
InchiKey: FBMSYYZACNSNGT-UHFFFAOYSA-N
Formula: C21H19N3O2
SMILES: O=C(Nc1ccc(N=Nc2ccccc2)cc1)OCCc1ccccc1
Mol. weight [g/mol]: 345.39
CAS: 95937-85-2

Physical Properties

Property code	Value	Unit	Source
hf	77.24	kJ/mol	Joback Method
hvap	92.09	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.893		Crippen Method
mcvol	268.550	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
tb	1040.56	K	Joback Method
tc	1304.08	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=C95937852&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature