P-phenyl azo carbanilic acid, cinnamyl ester

Inchi: InChI=1S/C22H19N3O2/c26-22(27-17-7-10-18-8-3-1-4-9-18)23-19-13-15-21(16-14-19)25
InchiKey: KHTDQWIGWSVYNA-WVLXALBKSA-N
Formula: C22H19N3O2
SMILES: O=C(Nc1ccc(N=Nc2ccccc2)cc1)OCC=Cc1ccccc1
Mol. weight [g/mol]: 357.41
CAS: 95166-23-7

Physical Properties

Property code	Value	Unit	Source
hf	173.82	kJ/mol	Joback Method
hvap	94.28	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	6.364		Crippen Method
mcvol	278.340	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
tb	1067.60	K	Joback Method
tc	1334.87	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=C95166237&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