P-phenylazo carbanilic acid, n-heptyl ester

Inchi: InChI=1S/C20H25N3O2/c1-2-3-4-5-9-16-25-20(24)21-17-12-14-19(15-13-17)23-22-18-10
InchiKey: GCLIEEGTFPJRCY-GHVJWSGMSA-N
Formula: C20H25N3O2
SMILES: CCCCCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 339.43
CAS: 94913-08-3

Physical Properties

Property code	Value	Unit	Source
hf	-138.65	kJ/mol	Joback Method
hvap	87.59	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	6.621		Crippen Method
mcvol	278.220	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
tb	991.00	K	Joback Method
tc	1229.23	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94913083&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