P-phenylazo carbanilic acid, n-octyl ester

Inchi: InChI=1S/C21H27N3O2/c1-2-3-4-5-6-10-17-26-21(25)22-18-13-15-20(16-14-18)24-23-19
InchiKey: UWMHYIKTIXVNSX-WCWDXBQESA-N
Formula: C21H27N3O2
SMILES: CCCCCCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 353.46
CAS: 95291-05-7

Physical Properties

Property code	Value	Unit	Source
hf	-159.29	kJ/mol	Joback Method
hvap	89.82	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	7.011		Crippen Method
mcvol	292.310	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
tb	1013.88	K	Joback Method
tc	1252.12	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95291057&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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