P-phenylazo carbanilic acid, n-undecyl ester

Inchi: InChI=1S/C24H33N3O2/c1-2-3-4-5-6-7-8-9-13-20-29-24(28)25-21-16-18-23(19-17-21)27
InchiKey: KMABDBDYQMWHMX-CYYJNZCTSA-N
Formula: C24H33N3O2
SMILES: CCCCCCCCCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 395.54
CAS: 95747-68-5

Physical Properties

Property code	Value	Unit	Source
hf	-221.21	kJ/mol	Joback Method
hvap	96.49	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	8.181		Crippen Method
mcvol	334.580	ml/mol	McGowan Method
pc	1055.51	kPa	Joback Method
tb	1082.52	K	Joback Method
tc	1326.53	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95747685&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