P-phenylazo carbanilic acid, n-nonyl ester

Inchi: InChI=1S/C22H29N3O2/c1-2-3-4-5-6-7-11-18-27-22(26)23-19-14-16-21(17-15-19)25-24-
InchiKey: CAMRBOHFBOHIER-OCOZRVBESA-N
Formula: C22H29N3O2
SMILES: CCCCCCCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 367.48
CAS: 95138-66-2

Physical Properties

Property code	Value	Unit	Source
hf	-179.93	kJ/mol	Joback Method
hvap	92.04	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	7.401		Crippen Method
mcvol	306.400	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
tb	1036.76	K	Joback Method
tc	1275.93	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=C95138662&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