P-phenylazo carbanilic acid, n-dodecyl ester

Inchi: InChI=1S/C25H35N3O2/c1-2-3-4-5-6-7-8-9-10-14-21-30-25(29)26-22-17-19-24(20-18-22
InchiKey: REQDTJIKQMTNTK-BYYHNAKLSA-N
Formula: C25H35N3O2
SMILES: CCCCCCCCCCCCOC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 409.56
CAS: 95961-99-2

Physical Properties

Property code	Value	Unit	Source
hf	-241.85	kJ/mol	Joback Method
hvap	98.72	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	8.571		Crippen Method
mcvol	348.670	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
tb	1105.40	K	Joback Method
tc	1353.44	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=C95961992&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