P-phenyl azo carbanilic acid, cedrol ester

Inchi: InChI=1S/C28H35N3O2/c1-19-10-15-23-26(2,3)24-18-28(19,23)17-16-27(24,4)33-25(32)
InchiKey: KVAHSFBEHKORJU-NVQSTNCTSA-N
Formula: C28H35N3O2
SMILES: CC1CCC2C(C)(C)C3CC12CCC3(C)OC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 445.60
CAS: 103306-68-9

Physical Properties

Property code	Value	Unit	Source
hf	-112.99	kJ/mol	Joback Method
hvap	101.10	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	8.282		Crippen Method
mcvol	358.360	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
tb	1189.51	K	Joback Method
tc	1466.37	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=C103306689&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