P-phenylazo carbanilic acid, santalol ester

Inchi: InChI=1S/C28H33N3O2/c1-19(8-7-15-27(2)20-16-24-25(17-20)28(24,27)3)18-33-26(32)2
InchiKey: YZHGYPCCSDHJCK-CLRLYFTESA-N
Formula: C28H33N3O2
SMILES: CC(=CCCC1(C)C2CC3C(C2)C31C)COC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 443.58
CAS: 107894-67-7

Physical Properties

Property code	Value	Unit	Source
hf	24.18	kJ/mol	Joback Method
hvap	101.91	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	8.059		Crippen Method
mcvol	354.060	ml/mol	McGowan Method
pc	1081.35	kPa	Joback Method
tb	1180.90	K	Joback Method
tc	1448.87	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107894677&Units=SI

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