

P-phenylazo carbanilic acid, bornyl ester

Inchi: InChI=1S/C23H27N3O2/c1-22(2)16-13-14-23(22,3)20(15-16)28-21(27)24-17-9-11-19(12)
InchiKey: CVSNPQASIXWELE-UHFFFAOYSA-N
Formula: C23H27N3O2
SMILES: CC1(C)C2CCC1(C)C(OC(=O)Nc1ccc(N=Nc3ccccc3)cc1)C2
Mol. weight [g/mol]: 377.48
CAS: 96369-27-6

Physical Properties

Property code	Value	Unit	Source
hf	-71.33	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.865		Crippen Method
mcvol	298.770	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
tb	1068.53	K	Joback Method
tc	1333.86	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C96369276&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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