

P-phenylazo carbanilic acid, 4-terpinenol ester

Inchi: InChI=1S/C23H27N3O2/c1-16(2)21-14-9-17(3)15-22(21)28-23(27)24-18-10-12-20(13-11)
InchiKey: KNGBJNQXPCNLFK-UHFFFAOYSA-N
Formula: C23H27N3O2
SMILES: CC1=CCC(C(C)C)C(OC(=O)Nc2ccc(N=Nc3ccccc3)cc2)C1
Mol. weight [g/mol]: 377.48

Physical Properties

Property code	Value	Unit	Source
hf	-125.56	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	7.031		Crippen Method
mcvol	305.330	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
tb	1078.22	K	Joback Method
tc	1338.07	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=B6002472&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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