

P-phenylazo carbanilic acid, 7,8-dihydrolinalool ester

Inchi: InChI=1S/C23H29N3O2/c1-5-23(4,17-9-10-18(2)3)28-22(27)24-19-13-15-21(16-14-19)26
InchiKey: BGJIGSTYOPRCHT-OCEACIFDSA-N
Formula: C23H29N3O2
SMILES: C=C(C)CCCC(C)(CC)OC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 379.50

Physical Properties

Property code	Value	Unit	Source
hf	-93.68	kJ/mol	Joback Method
hvap	92.38	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	7.566		Crippen Method
mcvol	316.190	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
tb	1052.97	K	Joback Method
tc	1300.07	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002475&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

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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