

P-phenyl azo carbanilic acid, linalyl ester

Inchi: InChI=1S/C23H27N3O2/c1-5-23(4,17-9-10-18(2)3)28-22(27)24-19-13-15-21(16-14-19)26
InchiKey: GAOZVVSFKAHRAN-UHFFFAOYSA-N
Formula: C23H27N3O2
SMILES: C=CC(C)(CCC=C(C)C)OC(=O)Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 377.48
CAS: 95439-22-8

Physical Properties

Property code	Value	Unit	Source
hf	23.54	kJ/mol	Joback Method
hvap	92.34	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	7.342		Crippen Method
mcvol	311.890	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
tb	1057.13	K	Joback Method
tc	1308.65	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=C95439228&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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