P-phenylazo carbanilic acid, tetrahydrolinalool ester

Inchi: InChI=1S/C23H31N3O2/c1-5-23(4,17-9-10-18(2)3)28-22(27)24-19-13-15-21(16-14-19)26

InchiKey: HFQXDQLQQDQPMA-OCEACIFDSA-N

Formula: C23H31N3O2

SMILES: CCC(C)(CCCC(C)C)OC(=O)Nc1ccc(N=Nc2ccccc2)cc1

Mol. weight [g/mol]: 381.51

CAS: 95293-43-9

Physical Properties

Property code	Value	Unit	Source
hf	-214.60	kJ/mol	Joback Method
hvap	92.58	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	7.645		Crippen Method
mcvol	320.490	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
tb	1055.97	K	Joback Method
tc	1301.86	K	Joback Method

Sources

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=C95293439&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from: