

M-toluidine, n-(p-methoxybenzylidene)-4-(p-methoxyphenylazo)

Inchi:	InChI=1S/C22H21N3O2/c1-16-14-19(23-15-17-4-9-20(26-2)10-5-17)8-13-22(16)25-24-18
InchiKey:	QGPNELIJUFWWCH-DPWLSMTKSA-N
Formula:	C22H21N3O2
SMILES:	COc1ccc(C=Nc2ccc(N=Nc3ccc(OC)cc3)c(C)c2)cc1
Mol. weight [g/mol]:	359.42
CAS:	13750-95-3

Physical Properties

Property code	Value	Unit	Source
hf	31.30	kJ/mol	Joback Method
hvap	88.85	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	6.178		Crippen Method
mcvol	282.640	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
tb	1073.44	K	Joback Method
tc	1340.62	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13750953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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