

p-Methoxybenzylidene p-phenylazoaniline

Other names:	p-Methoxybenzylidene p-phenylazoaniline N-(p-Anisylidene)-p-phenylazo aniline Aniline, N-(p-methoxybenzylidene)-p-(phenylazo)- Anisal-p-aminoazobenzene Benzenamine, N-((4-methoxyphenyl)methylene)-4-(phenylazo)- N-(p-Methoxybenzylidene)-p-(phenylazo)aniline 4-(4-Methoxybenzylidenamino)azobenzene N-(4-Methoxybenzylidene)-4-(phenylazo)aniline N-[(4-Methoxyphenyl)methylidene]-4-[phenyldiazenyl]aniline 4-(4-Methoxybenzylidenamino)azobenzene
Inchi:	InChI=1S/C20H17N3O/c1-24-20-13-7-16(8-14-20)15-21-17-9-11-19(12-10-17)23-22-18-5
InchiKey:	HLJXCFUTNROPTR-UHFFFAOYSA-N
Formula:	C20H17N3O
SMILES:	COc1ccc(C=Nc2ccc(N=Nc3ccccc3)cc2)cc1
Mol. weight [g/mol]:	315.38

Physical Properties

Property code	Value	Unit	Source
hf	436.66	kJ/mol	Cheméo Relay (1.0)
hvap	113.15	kJ/mol	Cheméo Relay (1.0)
ie	7.57	eV	Cheméo Relay (1.0)
log10ws	-5.72		Cheméo Relay (1.0)
logp	5.861		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
tb	723.46	K	Cheméo Relay (1.0)
tc	1002.74	K	Cheméo Relay (1.0)
tf	410.63	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C744661&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tf: Normal melting (fusion) point

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