

1-METHOXYBENZENE,-4-(4-METHOXYBENZYLIDENE)

Other names:	p-Methoxybenzylidene-(4-methoxyphenyl)-amine
Inchi:	InChI=1S/C15H15NO2/c1-17-14-7-3-12(4-8-14)11-16-13-5-9-15(18-2)10-6-13/h3-11H,1-
InchiKey:	ZDOHZYPZEUJYKN-UHFFFAOYSA-N
Formula:	C15H15NO2
SMILES:	COc1ccc(C=Nc2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	241.29

Physical Properties

Property code	Value	Unit	Source
hf	0.59	kJ/mol	Cheméo Relay (1.0)
hvap	92.04	kJ/mol	Cheméo Relay (1.0)
ie	7.40	eV	Cheméo Relay (1.0)
log10ws	-4.18		Cheméo Relay (1.0)
logp	3.454		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
rinpol	2315.00		NIST Webbook
tb	652.58	K	Cheméo Relay (1.0)
tc	873.39	K	Cheméo Relay (1.0)
tf	389.62	K	Cheméo Relay (1.0)

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1749082&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
r_{inpol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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