

p-Dimethylaminobenzylidene p-phenetidine

Inchi:	InChI=1S/C17H20N2O/c1-4-20-17-11-7-15(8-12-17)18-13-14-5-9-16(10-6-14)19(2)3/h5-
InchiKey:	ULZYQFCXFXYXBU-UHFFFAOYSA-N
Formula:	C17H20N2O
SMILES:	CCOc1ccc(N=Cc2ccc(N(C)C)cc2)cc1
Mol. weight [g/mol]:	268.36

Physical Properties

Property code	Value	Unit	Source
hf	78.36	kJ/mol	Cheméo Relay (1.0)
ie	6.73	eV	Cheméo Relay (1.0)
log10ws	-4.53		Cheméo Relay (1.0)
logp	3.902		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
tb	669.62	K	Cheméo Relay (1.0)
tf	403.87	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15484932&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.cheméo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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<https://www.cheméo.com/cid/18-753-6/p-Dimethylaminobenylidene-p-phenetidine.pdf>

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