

3-METHOXYDIPHENYLAMINE

Other names:	3-methoxy-N-phenylaniline 3-methoxy-N-phenylbenzenamine Benzenamine, 3-methoxy-N-phenyl- N-phenyl-m-anisidine
Inchi:	InChI=1S/C13H13NO/c1-15-13-9-5-8-12(10-13)14-11-6-3-2-4-7-11/h2-10,14H,1H3
InchiKey:	MKASXAGBWHIGCF-UHFFFAOYSA-N
Formula:	C13H13NO
SMILES:	COc1cccc(Nc2ccccc2)c1
Mol. weight [g/mol]:	199.25

Physical Properties

Property code	Value	Unit	Source
hf	49.73	kJ/mol	Cheméo Relay (1.0)
hfus	23.41	kJ/mol	Joback Method
hvap	82.52	kJ/mol	Cheméo Relay (1.0)
ie	7.27	eV	Cheméo Relay (1.0)
log10ws	-4.07		Cheméo Relay (1.0)
logp	3.439		Crippen Method
mcvol	162.360	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	611.62	K	Cheméo Relay (1.0)
tc	893.57	K	Cheméo Relay (1.0)
tf	321.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.39	J/mol×K	627.77	Joback Method
cpg	415.13	J/mol×K	667.75	Joback Method
cpg	429.70	J/mol×K	707.73	Joback Method
cpg	443.16	J/mol×K	747.71	Joback Method
cpg	455.54	J/mol×K	787.68	Joback Method
cpg	466.90	J/mol×K	827.66	Joback Method
cpg	477.29	J/mol×K	867.64	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubilities of 3-Methoxy-N-phenylaniline and 4-Methoxy-N-phenylaniline in Five Organic Solvents (285 K to 333.75 K): Joback Method:	https://www.doi.org/10.1021/je3001816
McGowan Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101166&Units=SI
Crippen Method:	https://en.wikipedia.org/wiki/Joback_method
	http://link.springer.com/article/10.1007/BF02311772
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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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