

N-benzyl-p-anisidine

Other names:	N-Benzyl-4-methoxyaniline
Inchi:	InChI=1S/C14H15NO/c1-16-14-9-7-13(8-10-14)15-11-12-5-3-2-4-6-12/h2-10,15H,11H2,1
InchiKey:	LIJJGMDKVVOEFT-UHFFFAOYSA-N
Formula:	C14H15NO
SMILES:	COc1ccc(NCc2ccccc2)cc1
Mol. weight [g/mol]:	213.28

Physical Properties

Property code	Value	Unit	Source
hf	65.45	kJ/mol	Cheméo Relay (1.0)
hfus	26.00	kJ/mol	Joback Method
hvap	87.13	kJ/mol	Cheméo Relay (1.0)
ie	7.39	eV	Cheméo Relay (1.0)
log10ws	-3.88		Cheméo Relay (1.0)
logp	3.307		Crippen Method
mcvol	176.450	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	620.47	K	Cheméo Relay (1.0)
tf	345.21	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.69	J/mol×K	650.65	Joback Method
cpg	465.95	J/mol×K	689.80	Joback Method
cpg	481.03	J/mol×K	728.96	Joback Method
cpg	494.97	J/mol×K	768.11	Joback Method
cpg	507.82	J/mol×K	807.26	Joback Method
cpg	519.64	J/mol×K	846.42	Joback Method
cpg	530.46	J/mol×K	885.57	Joback Method

Sources

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=C17377956&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

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
tf:	Normal melting (fusion) point

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