

Benzamide, 3-methoxy-N-methyl-

Inchi:	InChI=1S/C9H11NO2/c1-10-9(11)7-4-3-5-8(6-7)12-2/h3-6H,1-2H3,(H,10,11)
InchiKey:	QCUZSRZQGYWQHC-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CN=C(O)c1cccc(OC)c1
Mol. weight [g/mol]:	165.19

Physical Properties

Property code	Value	Unit	Source
hf	-216.05	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.630		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	628.14	K	Joback Method
tc	841.24	K	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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