

# Benzamide, N-(3-methylphenyl)-4-methoxy-

<b>Inchi:</b>	InChI=1S/C15H15NO2/c1-11-4-3-5-13(10-11)16-15(17)12-6-8-14(18-2)9-7-12/h3-10H,1-
<b>InchiKey:</b>	DOEUHYAIQRIZIY-UHFFFAOYSA-N
<b>Formula:</b>	C15H15NO2
<b>SMILES:</b>	COc1ccc(C(=O)Nc2cccc(C)c2)cc1
<b>Mol. weight [g/mol]:</b>	241.29

## Physical Properties

Property code	Value	Unit	Source
gf	136.45	kJ/mol	Joback Method
hf	-94.14	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Joback Method
hvap	70.45	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.256		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	2329.00		NIST Webbook
rinpol	2329.00		NIST Webbook
tb	732.38	K	Joback Method
tc	969.14	K	Joback Method
tf	461.51	K	Joback Method
vc	0.719	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.70	J/molxK	732.38	Joback Method
cpg	531.33	J/molxK	771.84	Joback Method
cpg	544.80	J/molxK	811.30	Joback Method
cpg	557.14	J/molxK	850.76	Joback Method
cpg	568.42	J/molxK	890.22	Joback Method
cpg	578.65	J/molxK	929.68	Joback Method
cpg	587.90	J/molxK	969.14	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U307495&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307495&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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