

# 2-Benzyloxy-6-methoxybenzonitrile

<b>Inchi:</b>	InChI=1S/C15H13NO2/c1-17-14-8-5-9-15(13(14)10-16)18-11-12-6-3-2-4-7-12/h2-9H,11H
<b>InchiKey:</b>	IQODCSAPOJQTCB-UHFFFAOYSA-N
<b>Formula:</b>	C15H13NO2
<b>SMILES:</b>	COc1cccc(OCc2ccccc2)c1C#N
<b>Mol. weight [g/mol]:</b>	239.27
<b>CAS:</b>	167832-66-8

## Physical Properties

Property code	Value	Unit	Source
gf	204.16	kJ/mol	Joback Method
hf	-2.37	kJ/mol	Joback Method
hfus	25.79	kJ/mol	Joback Method
hvap	70.16	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.146		Crippen Method
mcvol	187.810	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
tb	752.84	K	Joback Method
tc	993.83	K	Joback Method
tf	446.14	K	Joback Method
vc	0.722	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.55	J/molxK	752.84	Joback Method
cpg	511.89	J/molxK	793.00	Joback Method
cpg	524.12	J/molxK	833.17	Joback Method
cpg	535.26	J/molxK	873.33	Joback Method
cpg	545.34	J/molxK	913.50	Joback Method
cpg	554.38	J/molxK	953.66	Joback Method
cpg	562.40	J/molxK	993.83	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C167832668&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C167832668&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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