

# p-Octyloxybenzotrile

<b>Other names:</b>	4-n-Octyloxybenzotrile Benzotrile, 4-(octyloxy)- 4-octyloxybenzotrile
<b>Inchi:</b>	InChI=1S/C15H21NO/c1-2-3-4-5-6-7-12-17-15-10-8-14(13-16)9-11-15/h8-11H,2-7,12H2,
<b>InchiKey:</b>	GFNSBTARZPEIPN-UHFFFAOYSA-N
<b>Formula:</b>	C15H21NO
<b>SMILES:</b>	CCCCCCCCOc1ccc(C#N)cc1
<b>Mol. weight [g/mol]:</b>	231.33
<b>CAS:</b>	88374-55-4

## Physical Properties

Property code	Value	Unit	Source
gf	206.38	kJ/mol	Joback Method
hf	-95.21	kJ/mol	Joback Method
hfus	30.95	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.298		Crippen Method
mcvol	205.700	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
tb	698.76	K	Joback Method
tc	903.47	K	Joback Method
tf	384.97	K	Joback Method
vc	0.811	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.59	J/molxK	698.76	Joback Method
cpg	575.83	J/molxK	732.88	Joback Method
cpg	590.18	J/molxK	767.00	Joback Method
cpg	603.68	J/molxK	801.12	Joback Method
cpg	616.35	J/molxK	835.23	Joback Method
cpg	628.21	J/molxK	869.35	Joback Method

cpg

639.28

J/mol×K

903.47

Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	445.00 ± 1.00	K	0.30	NIST Webbook

## 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=C88374554&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88374554&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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