

# benzoic acid, 4-(dimethylamino)-, octyl ester

<b>Other names:</b>	octyl 4-(dimethylamino)benzoate OPABA (Octyl dimethyl para amino benzoic acid)
<b>Inchi:</b>	InChI=1S/C17H27NO2/c1-4-5-6-7-8-9-14-20-17(19)15-10-12-16(13-11-15)18(2)3/h10-13
<b>InchiKey:</b>	YAGMLECKUBJRNO-UHFFFAOYSA-N
<b>Formula:</b>	C17H27NO2
<b>SMILES:</b>	CCCCCCCCOC(=O)c1ccc(N(C)C)cc1
<b>Mol. weight [g/mol]:</b>	277.40

## Physical Properties

Property code	Value	Unit	Source
gf	71.90	kJ/mol	Joback Method
hf	-346.42	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.270		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	708.75	K	Joback Method
tc	901.43	K	Joback Method
tf	424.92	K	Joback Method
vc	0.921	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.28	J/molxK	708.75	Joback Method
cpg	712.76	J/molxK	740.86	Joback Method
cpg	729.25	J/molxK	772.98	Joback Method
cpg	744.78	J/molxK	805.09	Joback Method
cpg	759.38	J/molxK	837.20	Joback Method
cpg	773.09	J/molxK	869.32	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U401864&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U401864&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.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>

## 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>rinpol:</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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