

# m-Methoxybenzoic acid, octadecyl ester

<b>Inchi:</b>	InChI=1S/C26H44O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-29-26(27)24-20-
<b>InchiKey:</b>	UBVGQHYZUPQEPU-UHFFFAOYSA-N
<b>Formula:</b>	C26H44O3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)c1cccc(OC)c1
<b>Mol. weight [g/mol]:</b>	404.63
<b>CAS:</b>	56954-76-8

## Physical Properties

Property code	Value	Unit	Source
gf	-68.10	kJ/mol	Joback Method
hf	-731.93	kJ/mol	Joback Method
hfus	60.72	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.114		Crippen Method
mcvol	366.750	ml/mol	McGowan Method
pc	881.04	kPa	Joback Method
rinpol	2974.50		NIST Webbook
tb	924.65	K	Joback Method
tc	1132.03	K	Joback Method
tf	516.11	K	Joback Method
vc	1.425	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.64	J/molxK	924.65	Joback Method
cpg	1244.06	J/molxK	959.21	Joback Method
cpg	1262.05	J/molxK	993.78	Joback Method
cpg	1278.67	J/molxK	1028.34	Joback Method
cpg	1293.96	J/molxK	1062.90	Joback Method
cpg	1307.96	J/molxK	1097.47	Joback Method
cpg	1320.71	J/molxK	1132.03	Joback Method
dvisc	0.0003838	Paxs	516.11	Joback Method

dvisc	0.0001850	Paxs	584.20	Joback Method
dvisc	0.0001039	Paxs	652.29	Joback Method
dvisc	0.0000650	Paxs	720.38	Joback Method
dvisc	0.0000441	Paxs	788.47	Joback Method
dvisc	0.0000319	Paxs	856.56	Joback Method
dvisc	0.0000241	Paxs	924.65	Joback Method

## Sources

<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=C56954768&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56954768&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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