

# 3-(3-methoxy-4-hexyloxy-phenyl)-2-methyl-propionic acid, methyl ester

Inchi: CCCCCOc1ccc(CC(C)C(=O)OC)cc1OC  
InchiKey: BQEKLEUILOHYIH-UHFFFAOYSA-N

Formula: C18H28O4

SMILES: CCCCCOc1ccc(CC(C)C(=O)OC)cc1OC

Mol. weight [g/mol]: 308.41

## Physical Properties

Property code	Value	Unit	Source
gf	-252.53	kJ/mol	Joback Method
hf	-715.78	kJ/mol	Joback Method
hfus	37.28	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.006		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	2090.20		NIST Webbook
rinpol	2090.20		NIST Webbook
tb	768.57	K	Joback Method
tc	964.21	K	Joback Method
tf	445.70	K	Joback Method
vc	0.990	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.26	J/molxK	768.57	Joback Method
cpg	787.28	J/molxK	801.18	Joback Method
cpg	803.25	J/molxK	833.78	Joback Method
cpg	818.17	J/molxK	866.39	Joback Method
cpg	832.05	J/molxK	899.00	Joback Method
cpg	844.89	J/molxK	931.61	Joback Method
cpg	856.68	J/molxK	964.21	Joback Method
dvisc	0.0005942	Paxs	445.70	Joback Method

dvisc	0.0003180	Paxs	499.51	Joback Method
dvisc	0.0001922	Paxs	553.32	Joback Method
dvisc	0.0001270	Paxs	607.13	Joback Method
dvisc	0.0000898	Paxs	660.95	Joback Method
dvisc	0.0000669	Paxs	714.76	Joback Method
dvisc	0.0000519	Paxs	768.57	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=R157890&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R157890&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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