

# Methyl 7-(4-methoxyphenyl)noracadiene-7-carboxylate

Inchi:	InChI=1S/C16H16O3/c1-18-12-9-7-11(8-10-12)16(15(17)19-2)13-5-3-4-6-14(13)16/h3-10
InchiKey:	NGFBFVCPBCXHCJ-UHFFFAOYSA-N
Formula:	C16H16O3
SMILES:	<chem>COC(=O)C1(c2ccc(OC)cc2)C2C=CC=CC21</chem>
Mol. weight [g/mol]:	256.30
CAS:	32777-11-0

## Physical Properties

Property code	Value	Unit	Source
gf	3.82	kJ/mol	Joback Method
hf	-275.63	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.478		Crippen Method
mcvol	195.530	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	707.49	K	Joback Method
tc	944.25	K	Joback Method
tf	456.95	K	Joback Method
vc	0.741	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.45	J/molxK	707.49	Joback Method
cpg	567.17	J/molxK	746.95	Joback Method
cpg	583.02	J/molxK	786.41	Joback Method
cpg	598.20	J/molxK	825.87	Joback Method
cpg	612.89	J/molxK	865.33	Joback Method
cpg	627.28	J/molxK	904.79	Joback Method
cpg	641.55	J/molxK	944.25	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=C32777110&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C32777110&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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