

# Avenaciolide, 6-[2-(3-ethoxyphenyl)ethyl]-4-demethylene

Inchi:	InChI=1S/C16H18O5/c1-2-19-11-5-3-4-10(8-11)6-7-13-12-9-14(17)21-15(12)16(18)20-13
InchiKey:	FRNBJCMQOWSWFO-UMVBOHGHSA-N
Formula:	C16H18O5
SMILES:	CCOc1cccc(CCC2OC(=O)C3OC(=O)CC23)c1
Mol. weight [g/mol]:	290.31

## Physical Properties

Property code	Value	Unit	Source
gf	-246.21	kJ/mol	Joback Method
hf	-707.19	kJ/mol	Joback Method
hfus	40.15	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.875		Crippen Method
mvol	211.570	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	826.45	K	Joback Method
tc	1069.84	K	Joback Method
tf	545.43	K	Joback Method
vc	0.794	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.58	J/molxK	826.45	Joback Method
cpg	705.32	J/molxK	867.02	Joback Method
cpg	720.42	J/molxK	907.58	Joback Method
cpg	733.89	J/molxK	948.15	Joback Method
cpg	745.71	J/molxK	988.71	Joback Method
cpg	755.90	J/molxK	1029.28	Joback Method
cpg	764.43	J/molxK	1069.84	Joback Method

# 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=R565796&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R565796&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>

# 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>rinpola:</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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