

# 2(E),8(Z)-Matricaria ester

<b>Inchi:</b>	InChI=1S/C11H10O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3-4,9-10H,1-2H3/b4-3-,10-9+
<b>InchiKey:</b>	GXPDZHWFJLUFGY-PWGWRZEZSA-N
<b>Formula:</b>	C11H10O2
<b>SMILES:</b>	CC=CC#CC#CC=CC(=O)OC
<b>Mol. weight [g/mol]:</b>	174.20

## Physical Properties

Property code	Value	Unit	Source
gf	373.86	kJ/mol	Joback Method
hf	263.87	kJ/mol	Joback Method
hfus	33.68	kJ/mol	Joback Method
hvap	53.46	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.298		Crippen Method
mcvol	147.490	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinsol	1540.00		NIST Webbook
tb	553.69	K	Joback Method
tc	789.55	K	Joback Method
tf	487.93	K	Joback Method
vc	0.559	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.16	J/mol×K	553.69	Joback Method
cpg	318.50	J/mol×K	593.00	Joback Method
cpg	330.13	J/mol×K	632.31	Joback Method
cpg	341.07	J/mol×K	671.62	Joback Method
cpg	351.35	J/mol×K	710.93	Joback Method
cpg	361.04	J/mol×K	750.24	Joback Method
cpg	370.15	J/mol×K	789.55	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R634550&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R634550&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>
<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>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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