

# 8(Z)-2,3-Dihydromatricaria ester

<b>Inchi:</b>	InChI=1S/C11H12O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h3-4H,9-10H2,1-2H3/b4-3-
<b>InchiKey:</b>	SUBPZNAQAWTPJI-ARJAWSKDSA-N
<b>Formula:</b>	C11H12O2
<b>SMILES:</b>	CC=CC#CC#CCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	176.21

## Physical Properties

Property code	Value	Unit	Source
gf	293.64	kJ/mol	Joback Method
hf	146.65	kJ/mol	Joback Method
hfus	33.48	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.522		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1537.00		NIST Webbook
rinpol	1537.00		NIST Webbook
tb	549.53	K	Joback Method
tc	774.76	K	Joback Method
tf	493.01	K	Joback Method
vc	0.580	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.44	J/mol×K	549.53	Joback Method
cpg	338.42	J/mol×K	587.07	Joback Method
cpg	350.74	J/mol×K	624.61	Joback Method
cpg	362.41	J/mol×K	662.15	Joback Method
cpg	373.45	J/mol×K	699.69	Joback Method
cpg	383.89	J/mol×K	737.22	Joback Method
cpg	393.73	J/mol×K	774.76	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=R634590&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R634590&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>
<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>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>h vap:</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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