

(Z,E)-Matricaria ester

Inchi:	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-
InchiKey:	GXPDZHWFJLUFGY-YKNGABIKSA-N
Formula:	C11H10O2
SMILES:	<chem>CC=CC#CC#CC=CC(=O)OC</chem>
Mol. weight [g/mol]:	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
tb	553.69	K	Joback Method
tc	789.55	K	Joback Method
tf	487.93	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R632821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/79-118-4/Z-E-Matricaria-ester.pdf>

Generated by Cheméo on 2024-04-28 22:13:51.216056788 +0000 UTC m=+16631680.136634100.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.