(E,E)-Matricaria ester

Inchi: InChI=1S/C14H12O4/c1-3-13(15)18-12-10-8-6-4-5-7-9-11-14(16)17-2/h3,8-11H,1,12H2,2
InchiKey: IJYWDRVUCDHGHI-GFULKKFKSA-N
Formula: C14H12O4
SMILES: C=CC(=O)OCC=CC#CC#CC=CC(=O)OC
Mol. weight [g/mol]: 244.24

Physical Properties

Property code	Value	Unit	Source
gf	253.04	kJ/mol	Joback Method
hf	82.58	kJ/mol	Joback Method
hfus	42.96	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	1.008		Crippen Method
mcvol	192.900	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook
tb	695.30	K	Joback Method
tc	925.56	K	Joback Method
tf	592.14	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.43	J/mol×K	695.30	Joback Method
cpg	477.07	J/mol×K	733.68	Joback Method
cpg	488.91	J/mol×K	772.05	Joback Method
cpg	499.99	J/mol×K	810.43	Joback Method
cpg	510.35	J/mol×K	848.81	Joback Method
cpg	520.01	J/mol×K	887.19	Joback Method
cpg	529.02	J/mol×K	925.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R231151&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume