2(Z),8(Z)-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-RTAKVZRXSA-N
Formula: C11H10O2
SMILES: CC=CC#CC#CC=CC(=O)OC
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
rinpol	1551.00		NIST Webbook
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/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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R634565&Units=SI
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

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

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