p-mentha-1,8-dien-9-yl propanoate

Other names: 1,8(10)-p-Menthadien-9-yl propanoate
Inchi: InChI=1S/C13H20O2/c1-4-13(14)15-9-11(3)12-7-5-10(2)6-8-12/h5,12H,3-4,6-9H2,1-2H3
InchiKey: SCFWNSYNNIGDRT-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: C=C(COC(=O)CC)C1CC=C(C)CC1
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-51.27	kJ/mol	Joback Method
hf	-340.18	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.242		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1920.00		NIST Webbook
tb	593.38	K	Joback Method
tc	799.99	K	Joback Method
tf	313.37	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.77	J/mol×K	593.38	Joback Method
cpg	482.81	J/mol×K	627.82	Joback Method
cpg	499.86	J/mol×K	662.25	Joback Method
cpg	515.95	J/mol×K	696.69	Joback Method
cpg	531.11	J/mol×K	731.12	Joback Method

cpg	545.34	J/mol×K	765.56	Joback Method
cpg	558.68	J/mol×K	799.99	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=R320528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume