1,8(10)-p-Menthadien-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
hfus	22.29	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-3.26		Cheméo Relay (1.0)
logp	3.242		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
ripol	1920.00		NIST Webbook
ripol	1920.00		NIST Webbook
tb	538.10	K	Cheméo Relay (1.0)
tf	263.56	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R320528&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point