p-mentha-1(7),8-dien-2-yl acetate

Other names: menthadien-2-yl acetate, p-1(7),8
Inchi: InChI=1S/C12H18O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h11-12H,1,3,5-7H2,2,4H3
InchiKey: CCLNPVCMIJDJLR-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: C=C(C)C1CCC(=C)C(OC(C)=O)C1
Mol. weight [g/mol]: 194.27
CAS: 1134-96-9

Physical Properties

Property code	Value	Unit	Source
gf	-34.65	kJ/mol	Joback Method
hf	-301.95	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	51.15	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.850		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
ripol	1763.00		NIST Webbook
tb	560.85	K	Joback Method
tc	769.45	K	Joback Method
tf	298.26	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.55	J/mol×K	560.85	Joback Method
cpg	432.66	J/mol×K	595.62	Joback Method
cpg	449.82	J/mol×K	630.38	Joback Method
cpg	466.06	J/mol×K	665.15	Joback Method
cpg	481.39	J/mol×K	699.92	Joback Method
cpg	495.80	J/mol×K	734.69	Joback Method
cpg	509.32	J/mol×K	769.45	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=C1134969&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume