Methyl 8,11,13-Abietadien-18-oate

Inchi: InChI=1S/C21H30O2/c1-14(2)15-7-9-17-16(13-15)8-10-18-20(17,3)11-6-12-21(18,4)19(2
InchiKey: PGZCJOPTDHWYES-JBACZVJFSA-N
Formula: C21H30O2
SMILES: COC(=O)C1(C)CCCC2(C)c3ccc(C(C)C)cc3CCC12
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	61.34	kJ/mol	Joback Method
hf	-369.84	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	72.27	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.993		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2288.00		NIST Webbook
tb	810.20	K	Joback Method
tc	1044.45	K	Joback Method
tf	507.45	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.31	J/mol×K	810.20	Joback Method
cpg	879.62	J/mol×K	849.24	Joback Method
cpg	902.74	J/mol×K	888.28	Joback Method
cpg	925.96	J/mol×K	927.33	Joback Method
cpg	949.61	J/mol×K	966.37	Joback Method
cpg	973.97	J/mol×K	1005.41	Joback Method
cpg	999.36	J/mol×K	1044.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R20437&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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