Methyl 8,13-Abietadien-18-oate

Inchi: InChI=1S/C21H32O2/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: MEQSJWRGVQAVJY-JBACZVJFSA-N
Formula: C21H32O2
SMILES: COC(=O)C1(C)CCCC2(C)C3=C(C=C(C(C)C)CC3)CCC12
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	31.38	kJ/mol	Joback Method
hf	-427.62	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.439		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook
tb	811.04	K	Joback Method
tc	1043.59	K	Joback Method
tf	506.69	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.85	J/mol×K	811.04	Joback Method
cpg	908.00	J/mol×K	849.80	Joback Method
cpg	931.89	J/mol×K	888.56	Joback Method
cpg	955.82	J/mol×K	927.31	Joback Method
cpg	980.09	J/mol×K	966.07	Joback Method
cpg	1004.99	J/mol×K	1004.83	Joback Method
cpg	1030.82	J/mol×K	1043.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R20441&Units=SI

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