Methyl 8(14),13(15)-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: XLNYKQDSHLEWFW-AFUJVPCRSA-N
Formula: C21H32O2
SMILES: COC(=O)C1(C)CCCC2(C)C3CCC(=C(C)C)C=C3CCC12
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	52.32	kJ/mol	Joback Method
hf	-411.28	kJ/mol	Joback Method
hfus	25.16	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.439		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
tb	804.21	K	Joback Method
tc	1038.48	K	Joback Method
tf	488.05	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.02	J/mol×K	804.21	Joback Method
cpg	911.81	J/mol×K	843.25	Joback Method
cpg	936.26	J/mol×K	882.30	Joback Method
cpg	960.68	J/mol×K	921.34	Joback Method
cpg	985.40	J/mol×K	960.39	Joback Method
cpg	1010.72	J/mol×K	999.43	Joback Method
cpg	1036.95	J/mol×K	1038.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R20469&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

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