Methyl 13«beta»-Abieta-7,9(11)dien-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: HALJWOPQKXPVQL-HGWQEYRNSA-N
Formula: C21H32O2
SMILES: COC(=O)C1(C)CCCC2(C)C3=CCC(C(C)C)CC3=CCC12
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	33.30	kJ/mol	Joback Method
hf	-436.49	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.295		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2278.00		NIST Webbook
tb	801.39	K	Joback Method
tc	1033.26	K	Joback Method
tf	489.93	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.67	J/mol×K	801.39	Joback Method
cpg	911.14	J/mol×K	840.03	Joback Method
cpg	935.22	J/mol×K	878.68	Joback Method
cpg	959.20	J/mol×K	917.32	Joback Method
cpg	983.38	J/mol×K	955.97	Joback Method
cpg	1008.04	J/mol×K	994.61	Joback Method
cpg	1033.50	J/mol×K	1033.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R20366&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

Latest version available from:
https://www.chemeo.com/cid/14-998-9/Methyl-13-beta-Abieta-7-9-11-dien-18-oate.pdf
Generated by Cheméo on 2024-10-12 02:15:56.512148428 +0000 UTC m=+3280219.149117677.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.