Methyl abiet-7-en-18-oate

Inchi: InChI=1S/C21H34O2/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: YUBSLXLMZVQYAG-UHFFFAOYSA-N
Formula: C21H34O2
SMILES: COC(=O)C1(C)CCCC2(C)C3CCC(C(C)C)CC3=CCC12
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	5.26	kJ/mol	Joback Method
hf	-503.14	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.375		Crippen Method
mcvol	277.310	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
tb	792.58	K	Joback Method
tc	1022.06	K	Joback Method
tf	472.41	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.37	J/mol×K	792.58	Joback Method
cpg	942.05	J/mol×K	830.83	Joback Method
cpg	967.14	J/mol×K	869.07	Joback Method
cpg	991.94	J/mol×K	907.32	Joback Method
cpg	1016.73	J/mol×K	945.56	Joback Method
cpg	1041.78	J/mol×K	983.81	Joback Method
cpg	1067.39	J/mol×K	1022.06	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=B6009415&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume