Methyl 8(14),12-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: SGPKKYHABMKBPF-AFUJVPCRSA-N
Formula: C21H32O2
SMILES: COC(=O)C1(C)CCCC2(C)C3CC=C(C(C)C)C=C3CCC12
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	2264.00		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

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=R20455&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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