Methyl 8,15-Isopimaradien-18-oate

Inchi: InChI=1S/C21H32O2/c1-6-19(2)13-10-16-15(14-19)8-9-17-20(16,3)11-7-12-21(17,4)18(2
InchiKey: GTFNGUBYWRFHMR-NRDMVMEKSA-N
Formula: C21H32O2
SMILES: C=CC1(C)CCC2=C(CCC3C(C)(C(=O)OC)CCCC23C)C1
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	88.13	kJ/mol	Joback Method
hf	-348.32	kJ/mol	Joback Method
hfus	18.18	kJ/mol	Joback Method
hvap	69.28	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.439		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2158.00		NIST Webbook
tb	799.59	K	Joback Method
tc	1036.90	K	Joback Method
tf	526.31	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.99	J/mol×K	799.59	Joback Method
cpg	908.01	J/mol×K	839.14	Joback Method
cpg	934.29	J/mol×K	878.69	Joback Method
cpg	961.27	J/mol×K	918.24	Joback Method
cpg	989.38	J/mol×K	957.79	Joback Method
cpg	1019.06	J/mol×K	997.34	Joback Method
cpg	1050.73	J/mol×K	1036.90	Joback Method

Sources

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=R20491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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