methyl (E)-trans-«alpha»-2,3-epoxybergamota-2,10-dien-1

Inchi: InChI=1S/C16H24O3/c1-10(14(17)18-4)6-5-7-15(2)11-8-12(15)16(3)13(9-11)19-16/h6,11

InchiKey: YNLCLDZXTPYXSM-JEXNTIKSSA-N

Formula: C16H24O3

SMILES: COC(=O)C(C)=CCCC1(C)C2CC3OC3(C)C1C2

Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	3.42	kJ/mol	Joback Method
hf	-428.58	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	61.56	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.090		Crippen Method
mcvol	212.730	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
tb	679.85	K	Joback Method
tc	892.19	K	Joback Method
tf	446.43	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.52	J/mol×K	679.85	Joback Method
cpg	658.85	J/mol×K	715.24	Joback Method
cpg	676.54	J/mol×K	750.63	Joback Method
cpg	693.87	J/mol×K	786.02	Joback Method
cpg	711.10	J/mol×K	821.41	Joback Method
cpg	728.51	J/mol×K	856.80	Joback Method
cpg	746.37	J/mol×K	892.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233706&Units=SI

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