Methyl 7,11-di-epi-6,10-epoxybisabol-2-en-12-oate

Inchi: InChI=1S/C16H26O3/c1-11-7-9-16(10-8-11)12(2)5-6-14(19-16)13(3)15(17)18-4/h7,9,11-
InchiKey: GUKDPQPFRORGOO-WBNCRLLSSA-N
Formula: C16H26O3
SMILES: COC(=O)C(C)C1CCC(C)C2(C=CC(C)CC2)O1
Mol. weight [g/mol]: 266.38

Physical Properties

Property code	Value	Unit	Source
gf	-168.59	kJ/mol	Joback Method
hf	-608.51	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	63.70	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.335		Crippen Method
mcvol	223.590	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	693.17	K	Joback Method
tc	917.68	K	Joback Method
tf	388.27	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.80	J/mol×K	693.17	Joback Method
cpg	698.16	J/mol×K	730.59	Joback Method
cpg	719.27	J/mol×K	768.01	Joback Method
cpg	739.27	J/mol×K	805.42	Joback Method
cpg	758.27	J/mol×K	842.84	Joback Method
cpg	776.40	J/mol×K	880.26	Joback Method
cpg	793.80	J/mol×K	917.68	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=R503243&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