Methyl 6,10-epoxybisabol-3-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/h7,12-14
InchiKey: OLGPNLWRCFUIMD-BHTBLZRRSA-N
Formula: C16H26O3
SMILES: COC(=O)C(C)C1CCC(C)C2(CC=C(C)CC2)O1
Mol. weight [g/mol]: 266.38

Physical Properties

Property code	Value	Unit	Source
gf	-170.51	kJ/mol	Joback Method
hf	-599.64	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	64.67	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.480		Crippen Method
mcvol	223.590	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	702.82	K	Joback Method
tc	928.10	K	Joback Method
tf	405.03	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.75	J/mol×K	702.82	Joback Method
cpg	695.44	J/mol×K	740.37	Joback Method
cpg	715.95	J/mol×K	777.91	Joback Method
cpg	735.43	J/mol×K	815.46	Joback Method
cpg	754.00	J/mol×K	853.00	Joback Method
cpg	771.79	J/mol×K	890.55	Joback Method
cpg	788.92	J/mol×K	928.10	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=R503238&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