Bisabola-2,10-diene 1,9-oxide

Inchi: InChI=1S/C15H24O/c1-10(2)7-13-9-12(4)14-6-5-11(3)8-15(14)16-13/h7-8,12-15H,5-6,9H
InchiKey: SUZWJCBHQIOYCF-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C)=CC1CC(C)C2CCC(C)=CC2O1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	138.98	kJ/mol	Joback Method
hf	-250.91	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	54.38	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.103		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1596.00		NIST Webbook
rinpol	1596.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1988.00		NIST Webbook
tb	598.95	K	Joback Method
tc	817.71	K	Joback Method
tf	292.94	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.40	J/mol×K	598.95	Joback Method
cpg	563.52	J/mol×K	635.41	Joback Method
cpg	585.23	J/mol×K	671.87	Joback Method
cpg	605.60	J/mol×K	708.33	Joback Method
cpg	624.68	J/mol×K	744.79	Joback Method
cpg	642.54	J/mol×K	781.25	Joback Method

cpg	659.24	J/mol×K	817.71	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=R427431&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume