bisabolene oxide

Inchi: InChI=1S/C15H24O/c1-11(2)6-5-7-12(3)13-8-9-15(4)14(10-13)16-15/h6,13-14H,3,5,7-10
InchiKey: GCCYGVVSKKTGJQ-UHFFFAOYSA-N
Formula: C15H24O
SMILES: C=C(CCC=C(C)C)C1CCC2(C)OC2C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	236.46	kJ/mol	Joback Method
hf	-127.52	kJ/mol	Joback Method
hfus	27.83	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2038.00		NIST Webbook
tb	583.47	K	Joback Method
tc	794.07	K	Joback Method
tf	302.64	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.28	J/mol×K	583.47	Joback Method
cpg	550.93	J/mol×K	618.57	Joback Method
cpg	570.27	J/mol×K	653.67	Joback Method
cpg	588.50	J/mol×K	688.77	Joback Method
cpg	605.77	J/mol×K	723.87	Joback Method

cpg	622.27	J/mol×K	758.97	Joback Method
cpg	638.16	J/mol×K	794.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R195129&Units=SI
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

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