Bisabola-1,3,5,7,11-pentaene

Inchi: InChI=1S/C15H20/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h7-11H,1,5-6H2,2-4H3/b14-

InchiKey: ATHANBLXCHRFDY-AUWJEWJLSA-N

Formula: C15H20

SMILES: C=C(C)CCC=C(C)c1ccc(C)cc1

Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	329.16	kJ/mol	Joback Method
hf	95.20	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	51.37	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.755		Crippen Method
mcvol	189.850	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1576.00		NIST Webbook
tb	574.86	K	Joback Method
tc	786.70	K	Joback Method
tf	262.99	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.97	J/mol×K	574.86	Joback Method
cpg	471.01	J/mol×K	610.17	Joback Method
cpg	487.97	J/mol×K	645.47	Joback Method
cpg	503.90	J/mol×K	680.78	Joback Method
cpg	518.88	J/mol×K	716.09	Joback Method
cpg	532.96	J/mol×K	751.39	Joback Method
cpg	546.20	J/mol×K	786.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418447&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

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