Bisabola-1,3,5,7-tetraene

Inchi: InChI=1S/C15H22/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h7-12H,5-6H2,1-4H3/b14-7-
InchiKey: YKWOHCWVJMGYOF-AUWJEWJLSA-N
Formula: C15H22
SMILES: CC(=CCCC(C)C)c1ccc(C)cc1
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	247.43	kJ/mol	Joback Method
hf	-25.72	kJ/mol	Joback Method
hfus	23.63	kJ/mol	Joback Method
hvap	51.57	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.835		Crippen Method
mcvol	194.150	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1557.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1557.00		NIST Webbook
tb	577.86	K	Joback Method
tc	786.13	K	Joback Method
tf	263.71	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.13	J/mol×K	577.86	Joback Method
cpg	492.87	J/mol×K	612.57	Joback Method
cpg	510.53	J/mol×K	647.28	Joback Method
cpg	527.17	J/mol×K	682.00	Joback Method
cpg	542.83	J/mol×K	716.71	Joback Method
cpg	557.58	J/mol×K	751.42	Joback Method
cpg	571.47	J/mol×K	786.13	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=R411322&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume