Bisabola-1,3,5,7(14),11-pentaene

Inchi: InChI=1S/C15H20/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h8-11H,1,4-7H2,2-3H3
InchiKey: FRNIMXBIDKGTCS-UHFFFAOYSA-N
Formula: C15H20
SMILES: C=C(C)CCCC(=C)c1ccc(C)cc1
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	336.78	kJ/mol	Joback Method
hf	103.41	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	50.74	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.755		Crippen Method
mcvol	189.850	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1509.00		NIST Webbook
tb	567.38	K	Joback Method
tc	774.48	K	Joback Method
tf	266.31	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.61	J/mol×K	567.38	Joback Method
cpg	469.51	J/mol×K	601.90	Joback Method
cpg	486.37	J/mol×K	636.41	Joback Method
cpg	502.25	J/mol×K	670.93	Joback Method
cpg	517.20	J/mol×K	705.45	Joback Method
cpg	531.26	J/mol×K	739.97	Joback Method
cpg	544.50	J/mol×K	774.48	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=R418467&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