

Bisabola-1,3,5,7(14)-tetraene

Inchi:	InChI=1S/C15H22/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h8-12H,4-7H2,1-3H3
InchiKey:	OUOQVJYYZABQJT-UHFFFAOYSA-N
Formula:	C15H22
SMILES:	<chem>C=C(CCCC(C)C)c1ccc(C)cc1</chem>
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	255.05	kJ/mol	Joback Method
hf	-17.51	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.835		Crippen Method
mcvol	194.150	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinsol	1483.00		NIST Webbook
tb	570.38	K	Joback Method
tc	774.04	K	Joback Method
tf	267.03	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.55	J/mol×K	570.38	Joback Method
cpg	491.14	J/mol×K	604.32	Joback Method
cpg	508.70	J/mol×K	638.27	Joback Method
cpg	525.27	J/mol×K	672.21	Joback Method
cpg	540.90	J/mol×K	706.15	Joback Method
cpg	555.64	J/mol×K	740.10	Joback Method
cpg	569.52	J/mol×K	774.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411317&Units=SI

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
mccvol:	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

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