Caryophylla-4(12),8(13)-dien-5«beta»-ol

Inchi: InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h5,12-14,16H,1,6-9
InchiKey: DWUYGFWOANEJRE-ORJHTEBDSA-N
Formula: C15H24O
SMILES: C=C1CCC(O)C(C)=CCC2C1CC2(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	19.98	kJ/mol	Joback Method
hvap	92.09	kJ/mol	Cheméo Relay (1.0)
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1590.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1590.00		NIST Webbook
tb	578.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.12	J/mol×K	663.81	Joback Method
cpg	595.62	J/mol×K	698.64	Joback Method
cpg	614.14	J/mol×K	733.48	Joback Method
cpg	631.79	J/mol×K	768.31	Joback Method
cpg	648.66	J/mol×K	803.14	Joback Method
cpg	664.87	J/mol×K	837.98	Joback Method
cpg	680.52	J/mol×K	872.81	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R610638&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature