

Caryophylla-2(12),6(13)-dien-5-«beta»-ol

Other names:	caryophylla-2(12),6(13)-dien-5«beta»-ol (= caryophylladienol I) Caryophylla-2(12),6(13)-dien-5 «beta»-ol (Caryophylladienol I) Caryophylladienol I
Inchi:	InChI=1S/C15H24O/c1-10-6-8-14(16)11(2)5-7-13-12(10)9-15(13,3)4/h12-14,16H,1-2,5-9
InchiKey:	CIIOYPOMGIECX-RUXDESIVSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C(CC2(C)C)C(=C)CCC1O
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	17.99	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Cheméo Relay (1.0)
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1624.00		NIST Webbook
rinpol	1628.00		NIST Webbook
ripol	2324.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
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ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2316.00		NIST Webbook
tb	577.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.21	J/mol×K	658.83	Joback Method
cpg	594.89	J/mol×K	693.49	Joback Method
cpg	613.57	J/mol×K	728.16	Joback Method
cpg	631.35	J/mol×K	762.82	Joback Method
cpg	648.34	J/mol×K	797.48	Joback Method
cpg	664.64	J/mol×K	832.14	Joback Method
cpg	680.34	J/mol×K	866.81	Joback Method

Sources

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=R236765&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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