Caryophylladienol II

Other names:	Caryophylla-4(14),8(15)-dien-5«alpha»-ol
	Caryophylla-2(12),6(13)-dien-5-«alpha»-ol
	Caryophylla-4(14),8(15)-dien-5a-ol
	Caryophylla-2(12),6(13)-dien-5 «alpha»-ol (caryophylladienol II)
	caryophylla-2(12),6(13)-dien-5«alpha»-ol (= caryophylladienol II)
	Caryophylla-4(14),8(15)-dien-5«alpha»-ol (=Caryophylladienol II)
	«alpha»-Caryophylla-4(14),8(15)-dien-5-ol
	Caryophylla-2(12),6(13)-dien-5 a-ol (Caryophylladienol II)
	Caryophyll«alpha»-2(12),6(13)-dien-5- «alpha»-ol (=Caryophylladienol-II)
	5-«alpha»-Hydroxycaryophylla-4(12),8(13)-diene
	Caryophyll«alpha»-2(12)-6(13)-dien-5«alpha»-ol
	caryophylladienol II (caryophylla-2(12),6(13)-dien-5 -ol)
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:	CIIYOYPOMGIECX-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C(CC2(C)C)C(=C)CCC1O
Mol. weight [g/mol]:	220.35
CAS:	19431-79-9

Physical Properties

Property code	Value	Unit	Source
gf	84.85	kJ/mol	Joback Method
hf	-247.32	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1624.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1635.00		NIST Webbook

rinpol	1604.00	NIST Webbook
rinpol	1641.00	NIST Webbook
rinpol	1634.00	NIST Webbook
rinpol	1641.00	NIST Webbook
rinpol	1641.00	NIST Webbook
rinpol	1627.00	NIST Webbook
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rinpol	1638.00	NIST Webbook
rinpol	1630.00	NIST Webbook
rinpol	1615.00	NIST Webbook
rinpol	1643.00	NIST Webbook
rinpol	1656.00	NIST Webbook
rinpol	1623.00	NIST Webbook
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rinpol	1627.00	NIST Webbook
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ripol	2336.00		NIST Webbook
ripol	2285.00		NIST Webbook
ripol	2302.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2324.00		NIST Webbook
ripol	2324.00		NIST Webbook
tb	658.83	K	Joback Method
tc	866.81	K	Joback Method
tf	380.69	K	Joback Method
vc	0.733	m3/kmol	Joback Method

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

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=C19431799&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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