

caryophylladienol

Inchi:	InChI=1S/C15H24O/c1-10-5-6-14-13(9-15(14,3)4)11(2)8-12(16)7-10/h12-14,16H,1-2,5-9
InchiKey:	ASLIKDGYUZGYOV-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C(CC2(C)C)C(=C)CC(O)C1
Mol. weight [g/mol]:	220.35

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	1623.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1629.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2320.00		NIST Webbook
ripol	2316.00		NIST Webbook
tb	658.83	K	Joback Method
tc	866.81	K	Joback Method
tf	380.69	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R289353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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