

caryophyllan-2,6-«beta»-oxide

Other names:	Caryophyllane-2,6-«beta»-oxide
Inchi:	InChI=1S/C15H26O/c1-9-5-11-7-10(2)12-8-15(3,4)14(12)13(6-9)16-11/h9-14H,5-8H2,1-4
InchiKey:	NMNXPYBXLIGRGP-XBQBKKMYSA-N
Formula:	C15H26O
SMILES:	CC1CC2CC(C)C3CC(C)(C)C3C(C1)O2
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	98.92	kJ/mol	Joback Method
hf	-351.13	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	51.36	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.872		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1590.00		NIST Webbook
rinpol	1559.00		NIST Webbook
tb	584.14	K	Joback Method
tc	802.98	K	Joback Method
tf	335.58	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.79	J/mol×K	584.14	Joback Method
cpg	589.19	J/mol×K	620.61	Joback Method
cpg	613.03	J/mol×K	657.09	Joback Method
cpg	635.49	J/mol×K	693.56	Joback Method
cpg	656.71	J/mol×K	730.03	Joback Method
cpg	676.87	J/mol×K	766.51	Joback Method
cpg	696.11	J/mol×K	802.98	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=R181432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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