

10-Hydroxy-«beta»-caryophyllene

Inchi:	InChI=1S/C15H24O/c1-11-6-5-7-12(2)13-10-14(3,4)15(13,16)9-8-11/h6,13,16H,2,5,7-10H
InchiKey:	UROVCJWHLNVTHJ-YIBQGTJZSA-N
Formula:	C15H24O
SMILES:	<chem>C=C1CCC=C(C)CCC2(O)C1CC2(C)C</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	54.32	kJ/mol	Joback Method
hf	-249.67	kJ/mol	Joback Method
hfus	12.61	kJ/mol	Joback Method
hvap	64.85	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mvol	197.760	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
ripol	2363.00		NIST Webbook
tb	668.72	K	Joback Method
tc	885.02	K	Joback Method
tf	408.43	K	Joback Method
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.53	J/mol×K	668.72	Joback Method
cpg	589.55	J/mol×K	704.77	Joback Method
cpg	607.80	J/mol×K	740.82	Joback Method
cpg	625.49	J/mol×K	776.87	Joback Method
cpg	642.84	J/mol×K	812.92	Joback Method
cpg	660.04	J/mol×K	848.97	Joback Method
cpg	677.32	J/mol×K	885.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R560880&Units=SI

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

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