

«beta»-Cubeb-6-ol

Inchi:	InChI=1S/C15H24O/c1-9(2)12-6-5-11(4)14-8-7-10(3)13(14)15(12,14)16/h9,11-13,16H,3,
InchiKey:	WBVCJHZCJJPTSE-KNXMPVSZSA-N
Formula:	C15H24O
SMILES:	<chem>C=C1CCC23C(C)CCC(C(C)C)C2(O)C13</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	132.99	kJ/mol	Joback Method
hf	-224.16	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	62.42	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinsol	1521.00		NIST Webbook
tb	649.13	K	Joback Method
tc	854.53	K	Joback Method
tf	407.93	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.78	J/mol×K	649.13	Joback Method
cpg	589.92	J/mol×K	683.36	Joback Method
cpg	607.25	J/mol×K	717.60	Joback Method
cpg	624.01	J/mol×K	751.83	Joback Method
cpg	640.42	J/mol×K	786.06	Joback Method
cpg	656.72	J/mol×K	820.29	Joback Method
cpg	673.13	J/mol×K	854.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R398204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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