

6-epi-shyobunol

Other names:	elema-1,3-dien-6«alpha»-ol Epishiobunol
Inchi:	InChI=1S/C15H26O/c1-7-15(6)9-8-12(10(2)3)14(16)13(15)11(4)5/h7,10,12-14,16H,1,4,8
InchiKey:	WOULTTPZJDSDEI-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	<chem>C=CC1(C)CCC(C(C)C)C(O)C1C(=C)C</chem>
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	99.12	kJ/mol	Joback Method
hf	-260.83	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.798		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpola	1505.00		NIST Webbook
rinpola	1517.00		NIST Webbook
ripola	1925.00		NIST Webbook
ripola	1881.00		NIST Webbook
tb	633.36	K	Joback Method
tc	827.92	K	Joback Method
tf	305.71	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.93	J/mol×K	633.36	Joback Method
cpg	606.35	J/mol×K	665.79	Joback Method
cpg	624.82	J/mol×K	698.21	Joback Method
cpg	642.44	J/mol×K	730.64	Joback Method

cpg	659.29	J/mol×K	763.06	Joback Method
cpg	675.46	J/mol×K	795.49	Joback Method
cpg	691.04	J/mol×K	827.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C69350614&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
mvol:	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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