

Guaia-6,10(14)-dien-4«beta»-ol

Other names:	Guaia-6,10(14)-diene-4«beta»-ol
Inchi:	InChI=1S/C15H24O/c1-10(2)12-6-5-11(3)13-7-8-15(4,16)14(13)9-12/h9-10,13-14,16H,3,
InchiKey:	BUPJOLXWQXEJSQ-YMAMQOFZSA-N
Formula:	C15H24O
SMILES:	C=C1CCC(C(C)C)=CC2C1CCC2(C)O
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	69.47	kJ/mol	Joback Method
hf	-264.03	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1605.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2262.00		NIST Webbook
tb	663.77	K	Joback Method
tc	870.50	K	Joback Method
tf	373.05	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	572.06	J/mol×K	663.77	Joback Method
cpg	590.64	J/mol×K	698.22	Joback Method
cpg	608.29	J/mol×K	732.68	Joback Method
cpg	625.13	J/mol×K	767.13	Joback Method
cpg	641.29	J/mol×K	801.59	Joback Method
cpg	656.87	J/mol×K	836.04	Joback Method
cpg	671.99	J/mol×K	870.50	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=R201264&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
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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