

Guaia-6,10(14)-dien-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-RBSFLKMASA-N
Formula:	C15H24O
SMILES:	<chem>C=C1CCC(C(C)C)=CC2C1CCC2(C)O</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	17.49	kJ/mol	Joback Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
rinpol	1631.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R617575&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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