

cis-Guai-6-en-10-ol

Inchi:	InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)13(14)9-12/h9-11,13-14,16H,5-
InchiKey:	TUFHRGQKTXJXPF-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC(C)C1=CC2C(C)CCC2C(C)(O)CC1
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	8.68	kJ/mol	Joback Method
hf	-368.61	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1577.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	659.94	K	Joback Method
tc	865.11	K	Joback Method
tf	355.13	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.80	J/molxK	659.94	Joback Method
cpg	617.79	J/molxK	694.13	Joback Method
cpg	636.77	J/molxK	728.33	Joback Method
cpg	654.86	J/molxK	762.52	Joback Method
cpg	672.18	J/molxK	796.72	Joback Method
cpg	688.83	J/molxK	830.91	Joback Method
cpg	704.93	J/molxK	865.11	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=R198935&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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