

epimer of guaiol

Inchi:	InChI=1S/C15H26O/c1-10-5-7-12(15(3,4)16)9-14-11(2)6-8-13(10)14/h10-12,16H,5-9H2,1
InchiKey:	TWVJWDMOZJXUID-SRVKXCTJSA-N
Formula:	C15H26O
SMILES:	CC1CCC(C(C)(C)O)CC2=C1CCC2C
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	17.53	kJ/mol	Joback Method
hf	-378.45	kJ/mol	Joback Method
hfus	20.67	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
tb	666.56	K	Joback Method
tc	872.62	K	Joback Method
tf	365.41	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.73	J/molxK	666.56	Joback Method
cpg	689.07	J/molxK	838.28	Joback Method
cpg	673.77	J/molxK	803.93	Joback Method
cpg	657.45	J/molxK	769.59	Joback Method
cpg	640.04	J/molxK	735.25	Joback Method
cpg	621.49	J/molxK	700.90	Joback Method
cpg	703.40	J/molxK	872.62	Joback Method
dvisc	0.0000963	Paxs	666.56	Joback Method

dvisc	0.0001400	Paxs	616.37	Joback Method
dvisc	0.0002173	Paxs	566.18	Joback Method
dvisc	0.0003676	Paxs	515.99	Joback Method
dvisc	0.0006963	Paxs	465.79	Joback Method
dvisc	0.0015389	Paxs	415.60	Joback Method
dvisc	0.0042291	Paxs	365.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R324184&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/69-006-9/epimer-of-guaiol.pdf>

Generated by Cheméo on 2024-04-26 22:12:11.486388087 +0000 UTC m=+16458780.406965450.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.