Guaiol

Other names:	5-Azulenemethanol, 1,2,3,4,5,6,7,8-octahydro-«alpha»,«alpha»,3,8-tetramethyl-, [3S-(3«alpha»,5«alpha»,8«alpha»)]-
	Guai-1(5)-en-11-ol
	Champaca camphor
	Champacol
	Guaiac alcohol
	«alpha»-Guaiol
	2-((3S,8S)-1,2,3,4,5,6,7,8-octahydro-3,8-dimethylazulen-5-yl)propan-2-ol
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-SDDRHHMPSA-N
Formula:	C15H26O
SMILES:	CC1CCC(C(C)(C)O)CC2=C1CCC2C
Mol. weight [g/mol]:	222.37
CAS:	489-86-1

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	1588.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1588.00		NIST Webbook
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rinpol	1591.00		NIST Webbook
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ripol	2104.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2103.00		NIST Webbook
tb	666.56	K	Joback Method
tc	872.62	K	Joback Method
tf	365.41	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0042291	Pa×s	365.41	Joback Method
dvisc	0.0000963	Pa×s	666.56	Joback Method
dvisc	0.0001400	Pa×s	616.37	Joback Method
dvisc	0.0002173	Pa×s	566.18	Joback Method
dvisc	0.0003676	Pa×s	515.99	Joback Method
dvisc	0.0006963	Pa×s	465.79	Joback Method
dvisc	0.0015389	Pa×s	415.60	Joback Method
hvapt	62.20	kJ/mol	467.00	NIST Webbook

Sources

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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

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
hvapt: Enthalpy of vaporization at a given temperature
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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