

cis-guai-9-en-11-ol

Other names:	cis-Guaia-9-en-11-ol
Inchi:	InChI=1S/C15H26O/c1-10-5-7-12(15(3,4)16)9-14-11(2)6-8-13(10)14/h5,11-14,16H,6-9H2
InchiKey:	KIZQJEOCEXOJQJ-CRWXNKLISA-N
Formula:	C15H26O
SMILES:	CC1=CCC(C(C)(C)O)CC2C(C)CCC12
Mol. weight [g/mol]:	222.37
CAS:	69659-91-2

Physical Properties

Property code	Value	Unit	Source
gf	19.45	kJ/mol	Joback Method
hf	-387.32	kJ/mol	Joback Method
hfus	22.13	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1678.00		NIST Webbook
ripol	2265.00		NIST Webbook
ripol	2265.00		NIST Webbook
tb	656.91	K	Joback Method
tc	862.03	K	Joback Method
tf	348.65	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.31	J/molxK	656.91	Joback Method
cpg	623.77	J/molxK	691.10	Joback Method
cpg	642.97	J/molxK	725.28	Joback Method
cpg	660.98	J/molxK	759.47	Joback Method
cpg	677.85	J/molxK	793.66	Joback Method

cpg	693.63	J/molxK	827.84	Joback Method
cpg	708.40	J/molxK	862.03	Joback Method
dvisc	0.0055621	Paxs	348.65	Joback Method
dvisc	0.0019378	Paxs	400.03	Joback Method
dvisc	0.0008583	Paxs	451.40	Joback Method
dvisc	0.0004490	Paxs	502.78	Joback Method
dvisc	0.0002648	Paxs	554.16	Joback Method
dvisc	0.0001709	Paxs	605.53	Joback Method
dvisc	0.0001181	Paxs	656.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69659912&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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