

«gamma»-Guaiene

Inchi:	InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h9-12H,5-8H2,1-4H3/t11
InchiKey:	YLPOFTFBOIPYLE-RYUDHWPBXSA-N
Formula:	C15H24
SMILES:	CC(C)C1=CC2=C(CCC2C)C(C)CC1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	177.11	kJ/mol	Joback Method
hf	-156.10	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1511.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1761.00		NIST Webbook
tb	585.98	K	Joback Method
tc	802.43	K	Joback Method
tf	304.69	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.23	J/molxK	585.98	Joback Method
cpg	525.21	J/molxK	622.06	Joback Method
cpg	545.92	J/molxK	658.13	Joback Method
cpg	565.40	J/molxK	694.21	Joback Method
cpg	583.72	J/molxK	730.28	Joback Method
cpg	600.91	J/molxK	766.36	Joback Method

cpg	617.03	J/molxK	802.43	Joback Method
dvisc	0.0020981	Paxs	304.69	Joback Method
dvisc	0.0012209	Paxs	351.57	Joback Method
dvisc	0.0008070	Paxs	398.45	Joback Method
dvisc	0.0005820	Paxs	445.34	Joback Method
dvisc	0.0004467	Paxs	492.22	Joback Method
dvisc	0.0003590	Paxs	539.10	Joback Method
dvisc	0.0002988	Paxs	585.98	Joback Method

Sources

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=R320706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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