

cis-«beta»-Guaiene

Inchi:	InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h11-12H,5-9H2,1-4H3/t1
InchiKey:	GIBQERSGRNPMEH-RYUDHWPXSA-N
Formula:	C15H24
SMILES:	CC(C)=C1CCC(C)C2=C(C1)C(C)CC2
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	196.13	kJ/mol	Joback Method
hf	-130.89	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	51.98	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1495.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1694.00		NIST Webbook
tb	588.80	K	Joback Method
tc	808.19	K	Joback Method
tf	302.81	K	Joback Method
vc	0.728	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.31	J/mol×K	588.80	Joback Method
cpg	525.51	J/mol×K	625.37	Joback Method
cpg	546.40	J/mol×K	661.93	Joback Method
cpg	566.04	J/mol×K	698.50	Joback Method
cpg	584.49	J/mol×K	735.06	Joback Method
cpg	601.81	J/mol×K	771.63	Joback Method
cpg	618.07	J/mol×K	808.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R600329&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
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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