

Guaia-3,9-diene

Inchi:	InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h10,13H,5-9H2,1-4H3
InchiKey:	CVIGNZLXCQGQNR-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1=C2CCC(C)=C2CC(C(C)C)CC1
Mol. weight [g/mol]:	204.35
CAS:	489-83-8

Physical Properties

Property code	Value	Unit	Source
gf	175.19	kJ/mol	Joback Method
hf	-147.23	kJ/mol	Joback Method
hfus	18.77	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mvol	191.890	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1556.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	595.63	K	Joback Method
tc	813.11	K	Joback Method
tf	321.45	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.77	J/mol×K	595.63	Joback Method
cpg	523.96	J/mol×K	631.88	Joback Method
cpg	543.93	J/mol×K	668.12	Joback Method
cpg	562.72	J/mol×K	704.37	Joback Method
cpg	580.40	J/mol×K	740.62	Joback Method
cpg	597.01	J/mol×K	776.86	Joback Method
cpg	612.61	J/mol×K	813.11	Joback Method

dvisc	0.0020246	Paxs	321.45	Joback Method
dvisc	0.0011622	Paxs	367.15	Joback Method
dvisc	0.0007544	Paxs	412.84	Joback Method
dvisc	0.0005337	Paxs	458.54	Joback Method
dvisc	0.0004020	Paxs	504.24	Joback Method
dvisc	0.0003174	Paxs	549.93	Joback Method
dvisc	0.0002599	Paxs	595.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C489838&Units=SI
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

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

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