4,6-Guaiadiene

Inchi: InChI=1S/C15H22/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h9,11,14H,1,5-8H2,2-4H
InchiKey: UYWHJEPHKSZXQH-SBXXRYSUSA-N
Formula: C15H22
SMILES: C=C(C)C1=CC2=C(C)CCC2C(C)CC1
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	258.84	kJ/mol	Joback Method
hf	-35.18	kJ/mol	Joback Method
hfus	21.16	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.645		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
ripol	1720.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1720.00		NIST Webbook
tb	582.98	K	Joback Method
tc	803.24	K	Joback Method
tf	303.97	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.60	J/mol×K	582.98	Joback Method
cpg	502.93	J/mol×K	619.69	Joback Method
cpg	522.97	J/mol×K	656.40	Joback Method
cpg	541.78	J/mol×K	693.11	Joback Method
cpg	559.44	J/mol×K	729.82	Joback Method
cpg	575.99	J/mol×K	766.53	Joback Method

cpg	591.50	J/mol×K	803.24	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=R418214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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