Maali-1,3-diene

Inchi: InChI=1S/C15H22/c1-10-6-5-8-15(4)9-7-11-13(12(10)15)14(11,2)3/h5-6,8,11-13H,7,9H2,
InchiKey: MOKVGUFJAMQBQM-QPIMWOCDSA-N
Formula: C15H22
SMILES: CC1=CC=CC2(C)CCC3C(C12)C3(C)C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	257.36	kJ/mol	Joback Method
hf	-52.96	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	47.39	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.191		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	1351.00		NIST Webbook
tb	565.80	K	Joback Method
tc	793.56	K	Joback Method
tf	358.95	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.94	J/mol×K	565.80	Joback Method
cpg	505.80	J/mol×K	603.76	Joback Method
cpg	526.11	J/mol×K	641.72	Joback Method
cpg	545.16	J/mol×K	679.68	Joback Method
cpg	563.26	J/mol×K	717.64	Joback Method
cpg	580.73	J/mol×K	755.60	Joback Method
cpg	597.85	J/mol×K	793.56	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R430190&Units=SI

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