2,4,6-Megastimatriene

Inchi: InChI=1S/C13H20/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h7-10H,5-6H2,1-4H3/b12-9+
InchiKey: HZAZIPVYRJKZCP-FMIVXFBMSA-N
Formula: C13H20
SMILES: CCCC=C1C(C)=CC=CC1(C)C
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	173.29	kJ/mol	Joback Method
hf	-61.97	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
ripol	1643.00		NIST Webbook
ripol	1643.00		NIST Webbook
tb	526.57	K	Joback Method
tc	735.76	K	Joback Method
tf	291.95	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.01	J/mol×K	526.57	Joback Method
cpg	411.94	J/mol×K	561.43	Joback Method
cpg	428.81	J/mol×K	596.30	Joback Method
cpg	444.72	J/mol×K	631.16	Joback Method
cpg	459.78	J/mol×K	666.03	Joback Method
cpg	474.10	J/mol×K	700.89	Joback Method
cpg	487.80	J/mol×K	735.76	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=R344599&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume