2,2,6,7-tetramethylbicyclo[4.3.0]nona-4,7,9(1)-trien

Inchi: InChI=1S/C13H18/c1-10-6-7-11-12(2,3)8-5-9-13(10,11)4/h5-7,9H,8H2,1-4H3
InchiKey: XOFDOXJFXCEFDE-UHFFFAOYSA-N
Formula: C13H18
SMILES: CC1=CC=C2C(C)(C)CC=CC12C
Mol. weight [g/mol]: 174.28

Physical Properties

Property code	Value	Unit	Source
gf	203.42	kJ/mol	Joback Method
hf	-3.65	kJ/mol	Joback Method
hfus	9.69	kJ/mol	Joback Method
hvap	44.77	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.865		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1150.00		NIST Webbook
rinpol	1200.00		NIST Webbook
ripol	1461.00		NIST Webbook
tb	531.05	K	Joback Method
tc	762.04	K	Joback Method
tf	336.71	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.67	J/mol×K	531.05	Joback Method
cpg	398.13	J/mol×K	569.55	Joback Method
cpg	415.13	J/mol×K	608.05	Joback Method
cpg	430.96	J/mol×K	646.54	Joback Method
cpg	445.88	J/mol×K	685.04	Joback Method
cpg	460.18	J/mol×K	723.54	Joback Method
cpg	474.13	J/mol×K	762.04	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=R54915&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume