1,4,4,7a-tetramethyl-4,5-dihydroindene

Inchi: InChI=1S/C13H18/c1-9-5-6-11-12(9)10(2)7-8-13(11,3)4/h5-7,9H,8H2,1-4H3
InchiKey: VZRXNBZXHYOPOV-UHFFFAOYSA-N
Formula: C13H18
SMILES: CC1=CCC(C)(C)C2=C1C(C)C=C2
Mol. weight [g/mol]: 174.28

Physical Properties

Property code	Value	Unit	Source
gf	199.28	kJ/mol	Joback Method
hf	-30.36	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	46.59	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.865		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1199.00		NIST Webbook
ripol	1432.00		NIST Webbook
tb	535.79	K	Joback Method
tc	758.43	K	Joback Method
tf	325.33	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.52	J/mol×K	535.79	Joback Method
cpg	398.73	J/mol×K	572.90	Joback Method
cpg	415.73	J/mol×K	610.00	Joback Method
cpg	431.68	J/mol×K	647.11	Joback Method
cpg	446.71	J/mol×K	684.21	Joback Method
cpg	460.99	J/mol×K	721.32	Joback Method
cpg	474.66	J/mol×K	758.43	Joback Method

Sources

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=R238043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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