trans-1-trans-4-hexadienyl-cyclopropane

Inchi: InChI=1S/C9H14/c1-2-3-4-5-6-9-7-8-9/h2-3,5-6,9H,4,7-8H2,1H3/b3-2+,6-5+
InchiKey: AGEOFELTLBOAMI-ZIMISOLQSA-N
Formula: C9H14
SMILES: CC=CCC=CC1CC1
Mol. weight [g/mol]: 122.21

Physical Properties

Property code	Value	Unit	Source
gf	246.09	kJ/mol	Joback Method
hf	78.15	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	35.46	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	936.50		NIST Webbook
rinpol	936.80		NIST Webbook
tb	420.38	K	Joback Method
tc	615.43	K	Joback Method
tf	198.97	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.08	J/mol×K	420.38	Joback Method
cpg	243.37	J/mol×K	452.89	Joback Method
cpg	257.68	J/mol×K	485.40	Joback Method
cpg	271.08	J/mol×K	517.90	Joback Method
cpg	283.64	J/mol×K	550.41	Joback Method
cpg	295.40	J/mol×K	582.92	Joback Method
cpg	306.42	J/mol×K	615.43	Joback Method
dvisc	0.0013080	Pa×s	198.97	Joback Method

dvisc	0.0008196	Pa×s	235.87	Joback Method
dvisc	0.0005828	Pa×s	272.77	Joback Method
dvisc	0.0004495	Pa×s	309.67	Joback Method
dvisc	0.0003664	Pa×s	346.58	Joback Method
dvisc	0.0003106	Pa×s	383.48	Joback Method
dvisc	0.0002711	Pa×s	420.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R138057&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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