

1-Methyl-trans-2-(trans-2,4-pentdienyl)-cycloprop

Inchi:	InChI=1S/C9H14/c1-3-4-5-6-9-7-8(9)2/h3-5,8-9H,1,6-7H2,2H3/b5-4+/t8-,9-/m1/s1
InchiKey:	LHQTUIQDWWUYAA-HOMPQPGZSA-N
Formula:	C9H14
SMILES:	C=CC=CCC1CC1C
Mol. weight [g/mol]:	122.21

Physical Properties

Property code	Value	Unit	Source
gf	246.00	kJ/mol	Joback Method
hf	66.02	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	34.52	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.775		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	885.40		NIST Webbook
rinpol	885.40		NIST Webbook
rinpol	884.20		NIST Webbook
tb	408.23	K	Joback Method
tc	597.26	K	Joback Method
tf	198.05	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.51	J/molxK	408.23	Joback Method
cpg	242.73	J/molxK	439.73	Joback Method
cpg	257.09	J/molxK	471.24	Joback Method
cpg	270.64	J/molxK	502.74	Joback Method
cpg	283.42	J/molxK	534.25	Joback Method
cpg	295.47	J/molxK	565.75	Joback Method
cpg	306.84	J/molxK	597.26	Joback Method

dvisc	0.0006536	Paxs	198.05	Joback Method
dvisc	0.0005184	Paxs	233.08	Joback Method
dvisc	0.0004368	Paxs	268.11	Joback Method
dvisc	0.0003829	Paxs	303.14	Joback Method
dvisc	0.0003450	Paxs	338.17	Joback Method
dvisc	0.0003169	Paxs	373.20	Joback Method
dvisc	0.0002954	Paxs	408.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R137574&Units=SI

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

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