

1-(1-Ethyenyl)-cis-2-(trans-2-butenyl)-cyclopropane

Inchi:	InChI=1S/C9H14/c1-3-5-6-9-7-8(9)4-2/h3-5,8-9H,2,6-7H2,1H3/b5-3+/t8-,9+/m1/s1
InchiKey:	LQRHENSISHISOYSH-ZHBVTVBMSA-N
Formula:	C9H14
SMILES:	C=CC1CC1CC=CC
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	892.10		NIST Webbook
rinpol	891.20		NIST Webbook
rinpol	892.10		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/mol×K	408.23	Joback Method
cpg	242.73	J/mol×K	439.73	Joback Method
cpg	257.09	J/mol×K	471.24	Joback Method
cpg	270.64	J/mol×K	502.74	Joback Method
cpg	283.42	J/mol×K	534.25	Joback Method
cpg	295.47	J/mol×K	565.75	Joback Method
cpg	306.84	J/mol×K	597.26	Joback Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136962&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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