

1-methyl-trans-2-(trans-3-pentenyl)-cyclopropane

Inchi:	InChI=1S/C9H16/c1-3-4-5-6-9-7-8(9)2/h3-4,8-9H,5-7H2,1-2H3/b4-3+/t8-,9-/m1/s1
InchiKey:	BRJAZMJACNNPEV-HUGTUPKYSA-N
Formula:	C9H16
SMILES:	CC=CCCC1CC1C
Mol. weight [g/mol]:	124.22

Physical Properties

Property code	Value	Unit	Source
gf	158.16	kJ/mol	Joback Method
hf	-59.41	kJ/mol	Joback Method
hfus	18.47	kJ/mol	Joback Method
hvap	35.19	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.999		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	860.50		NIST Webbook
rinpol	862.40		NIST Webbook
rinpol	861.80		NIST Webbook
tb	411.55	K	Joback Method
tc	596.57	K	Joback Method
tf	199.81	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.05	J/molxK	411.55	Joback Method
cpg	258.79	J/molxK	442.39	Joback Method
cpg	273.72	J/molxK	473.22	Joback Method
cpg	287.86	J/molxK	504.06	Joback Method
cpg	301.26	J/molxK	534.90	Joback Method
cpg	313.96	J/molxK	565.74	Joback Method
cpg	325.99	J/molxK	596.57	Joback Method

dvisc	0.0007918	Paxs	199.81	Joback Method
dvisc	0.0005994	Paxs	235.10	Joback Method
dvisc	0.0004879	Paxs	270.39	Joback Method
dvisc	0.0004165	Paxs	305.68	Joback Method
dvisc	0.0003674	Paxs	340.97	Joback Method
dvisc	0.0003318	Paxs	376.26	Joback Method
dvisc	0.0003049	Paxs	411.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R137594&Units=SI
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

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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