

trans-4-hexenyl-cyclopropane

Inchi:	InChI=1S/C9H16/c1-2-3-4-5-6-9-7-8-9/h2-3,9H,4-8H2,1H3/b3-2+
InchiKey:	WKWFRAVGNCBHOW-NSCUHMNNSA-N
Formula:	C9H16
SMILES:	CC=CCCC1CC1
Mol. weight [g/mol]:	124.22

Physical Properties

Property code	Value	Unit	Source
gf	165.87	kJ/mol	Joback Method
hf	-39.07	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	35.50	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpola	913.20		NIST Webbook
rinpola	911.80		NIST Webbook
rinpola	914.60		NIST Webbook
rinpola	913.20		NIST Webbook
tb	416.22	K	Joback Method
tc	601.73	K	Joback Method
tf	204.05	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.01	J/molxK	416.22	Joback Method
cpg	312.36	J/molxK	570.81	Joback Method
cpg	300.02	J/molxK	539.90	Joback Method
cpg	286.95	J/molxK	508.98	Joback Method
cpg	273.12	J/molxK	478.06	Joback Method
cpg	258.49	J/molxK	447.14	Joback Method

cpg	324.03	J/mol×K	601.73	Joback Method
dvisc	0.0003225	Paxs	416.22	Joback Method
dvisc	0.0003702	Paxs	380.86	Joback Method
dvisc	0.0004371	Paxs	345.50	Joback Method
dvisc	0.0005360	Paxs	310.13	Joback Method
dvisc	0.0006928	Paxs	274.77	Joback Method
dvisc	0.0009660	Paxs	239.41	Joback Method
dvisc	0.0015112	Paxs	204.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R138191&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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