

5-hexenyl-cyclopropane

Other names:	Cyclopropane, 5-hexenyl
Inchi:	InChI=1S/C9H16/c1-2-3-4-5-6-9-7-8-9/h2,9H,1,3-8H2
InchiKey:	NGWWCTFUAWVMRV-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	C=CCCCC1CC1
Mol. weight [g/mol]:	124.22

Physical Properties

Property code	Value	Unit	Source
gf	173.49	kJ/mol	Joback Method
hf	-30.86	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	34.87	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	893.70		NIST Webbook
rinpol	899.50		NIST Webbook
rinpol	897.40		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	895.34		NIST Webbook
rinpol	895.20		NIST Webbook
rinpol	895.34		NIST Webbook
tb	408.74	K	Joback Method
tc	589.00	K	Joback Method
tf	207.37	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.09	J/mol×K	408.74	Joback Method
cpg	257.21	J/mol×K	438.78	Joback Method

cpg	271.56	J/mol×K	468.83	Joback Method
cpg	285.18	J/mol×K	498.87	Joback Method
cpg	298.08	J/mol×K	528.91	Joback Method
cpg	310.32	J/mol×K	558.96	Joback Method
cpg	321.92	J/mol×K	589.00	Joback Method
dvisc	0.0014737	Paxs	207.37	Joback Method
dvisc	0.0010002	Paxs	240.93	Joback Method
dvisc	0.0007464	Paxs	274.49	Joback Method
dvisc	0.0005936	Paxs	308.06	Joback Method
dvisc	0.0004939	Paxs	341.62	Joback Method
dvisc	0.0004246	Paxs	375.18	Joback Method
dvisc	0.0003743	Paxs	408.74	Joback Method

Sources

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=R2029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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