

Pentanal, 5-(methylenecyclopropyl)-

Other names:	5-(Methylenecyclopropyl)pentanal
Inchi:	InChI=1S/C9H14O/c1-8-7-9(8)5-3-2-4-6-10/h6,9H,1-5,7H2
InchiKey:	XBTXVMOVNAXWNM-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	C=C1CC1CCCC=O
Mol. weight [g/mol]:	138.21

Physical Properties

Property code	Value	Unit	Source
gf	39.21	kJ/mol	Joback Method
hf	-157.63	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	459.88	K	Joback Method
tc	644.42	K	Joback Method
tf	264.81	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.62	J/molxK	459.88	Joback Method
cpg	281.55	J/molxK	490.64	Joback Method
cpg	293.82	J/molxK	521.39	Joback Method
cpg	305.47	J/molxK	552.15	Joback Method
cpg	316.53	J/molxK	582.90	Joback Method
cpg	327.01	J/molxK	613.66	Joback Method
cpg	336.96	J/molxK	644.42	Joback Method
dvisc	0.0016954	Paxs	264.81	Joback Method
dvisc	0.0012791	Paxs	297.32	Joback Method

dvisc	0.0010202	Paxs	329.83	Joback Method
dvisc	0.0008474	Paxs	362.35	Joback Method
dvisc	0.0007257	Paxs	394.86	Joback Method
dvisc	0.0006363	Paxs	427.37	Joback Method
dvisc	0.0005684	Paxs	459.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U158491&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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