

1,3-Cyclopentadiene, 5-butyl

Inchi:	InChI=1S/C9H14/c1-2-3-6-9-7-4-5-8-9/h4-5,7-9H,2-3,6H2,1H3
InchiKey:	LDZPPZNDWQFMAU-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	CCCCC1C=CC=C1
Mol. weight [g/mol]:	122.21

Physical Properties

Property code	Value	Unit	Source
gf	121.37	kJ/mol	Joback Method
hf	-53.05	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	36.47	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1144.50		NIST Webbook
ripol	1144.50		NIST Webbook
tb	418.92	K	Joback Method
tc	613.95	K	Joback Method
tf	203.61	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.75	J/molxK	418.92	Joback Method
cpg	243.90	J/molxK	451.42	Joback Method
cpg	258.26	J/molxK	483.93	Joback Method
cpg	271.86	J/molxK	516.43	Joback Method
cpg	284.74	J/molxK	548.94	Joback Method
cpg	296.91	J/molxK	581.44	Joback Method

cpg	308.42	J/mol×K	613.95	Joback Method
dvisc	0.0025781	Paxs	203.61	Joback Method
dvisc	0.0013518	Paxs	239.50	Joback Method
dvisc	0.0008387	Paxs	275.38	Joback Method
dvisc	0.0005809	Paxs	311.26	Joback Method
dvisc	0.0004341	Paxs	347.15	Joback Method
dvisc	0.0003426	Paxs	383.03	Joback Method
dvisc	0.0002816	Paxs	418.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40895&Units=SI

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

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