

1,3-Cyclopentadiene, 2-butyl

Inchi:	InChI=1S/C9H14/c1-2-3-6-9-7-4-5-8-9/h4,7-8H,2-3,5-6H2,1H3
InchiKey:	HILJWHUIEBFFEW-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	CCCCC1=CCC=C1
Mol. weight [g/mol]:	122.21

Physical Properties

Property code	Value	Unit	Source
gf	119.45	kJ/mol	Joback Method
hf	-44.18	kJ/mol	Joback Method
hfus	13.98	kJ/mol	Joback Method
hvap	37.44	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.063		Crippen Method
mvol	118.210	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	913.00		NIST Webbook
ripol	1108.20		NIST Webbook
tb	428.57	K	Joback Method
tc	625.48	K	Joback Method
tf	220.37	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.94	J/mol×K	428.57	Joback Method
cpg	244.32	J/mol×K	461.39	Joback Method
cpg	257.93	J/mol×K	494.21	Joback Method
cpg	270.82	J/mol×K	527.03	Joback Method
cpg	283.01	J/mol×K	559.85	Joback Method
cpg	294.54	J/mol×K	592.66	Joback Method
cpg	305.43	J/mol×K	625.48	Joback Method
dvisc	0.0029321	Paxs	220.37	Joback Method

dvisc	0.0015112	Paxs	255.07	Joback Method
dvisc	0.0009129	Paxs	289.77	Joback Method
dvisc	0.0006142	Paxs	324.47	Joback Method
dvisc	0.0004461	Paxs	359.17	Joback Method
dvisc	0.0003428	Paxs	393.87	Joback Method
dvisc	0.0002749	Paxs	428.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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