

1,3-Cyclopentadiene, 2-(1-methylethyl)

Inchi:	InChI=1S/C8H12/c1-7(2)8-5-3-4-6-8/h3,5-7H,4H2,1-2H3
InchiKey:	IQMSPGKWQJYFX-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	CC(C)C1=CCC=C1
Mol. weight [g/mol]:	108.18

Physical Properties

Property code	Value	Unit	Source
gf	108.59	kJ/mol	Joback Method
hf	-28.82	kJ/mol	Joback Method
hfus	7.87	kJ/mol	Joback Method
hvap	34.83	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.529		Crippen Method
mvol	104.120	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	785.00		NIST Webbook
tb	405.25	K	Joback Method
tc	608.95	K	Joback Method
tf	194.10	K	Joback Method
vc	0.392	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.96	J/molxK	405.25	Joback Method
cpg	203.61	J/molxK	439.20	Joback Method
cpg	216.51	J/molxK	473.15	Joback Method
cpg	228.69	J/molxK	507.10	Joback Method
cpg	240.17	J/molxK	541.05	Joback Method
cpg	250.99	J/molxK	575.00	Joback Method
cpg	261.19	J/molxK	608.95	Joback Method
dvisc	0.0040067	Paxs	194.10	Joback Method
dvisc	0.0017923	Paxs	229.29	Joback Method

dvisc	0.0009932	Paxs	264.48	Joback Method
dvisc	0.0006322	Paxs	299.68	Joback Method
dvisc	0.0004425	Paxs	334.87	Joback Method
dvisc	0.0003315	Paxs	370.06	Joback Method
dvisc	0.0002611	Paxs	405.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40788&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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