

1,3-Cyclopentadiene, 1-hexyl

Inchi:	InChI=1S/C11H18/c1-2-3-4-5-8-11-9-6-7-10-11/h6-7,9H,2-5,8,10H2,1H3
InchiKey:	WVYLDZGPTDJRJS-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	CCCCCCC1=CC=CC1
Mol. weight [g/mol]:	150.26

Physical Properties

Property code	Value	Unit	Source
gf	136.29	kJ/mol	Joback Method
hf	-85.46	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.843		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1111.00		NIST Webbook
ripol	1311.80		NIST Webbook
tb	474.33	K	Joback Method
tc	666.96	K	Joback Method
tf	242.91	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.14	J/molxK	474.33	Joback Method
cpg	332.41	J/molxK	506.44	Joback Method
cpg	347.84	J/molxK	538.54	Joback Method
cpg	362.47	J/molxK	570.65	Joback Method
cpg	376.34	J/molxK	602.75	Joback Method
cpg	389.47	J/molxK	634.86	Joback Method
cpg	401.90	J/molxK	666.96	Joback Method
dvisc	0.0033452	Paxs	242.91	Joback Method

dvisc	0.0016415	Paxs	281.48	Joback Method
dvisc	0.0009563	Paxs	320.05	Joback Method
dvisc	0.0006258	Paxs	358.62	Joback Method
dvisc	0.0004446	Paxs	397.19	Joback Method
dvisc	0.0003356	Paxs	435.76	Joback Method
dvisc	0.0002652	Paxs	474.33	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=R40738&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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