

1,3-Cyclopentadiene, 5-octyl

Inchi:	InChI=1S/C13H22/c1-2-3-4-5-6-7-10-13-11-8-9-12-13/h8-9,11-13H,2-7,10H2,1H3
InchiKey:	KXVQRALPVVEFPC-UHFFFAOYSA-N
Formula:	C13H22
SMILES:	CCCCCCCCC1C=CC=C1
Mol. weight [g/mol]:	178.31

Physical Properties

Property code	Value	Unit	Source
gf	155.05	kJ/mol	Joback Method
hf	-135.61	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	45.37	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.479		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinsol	1328.00		NIST Webbook
tb	510.44	K	Joback Method
tc	697.26	K	Joback Method
tf	248.69	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.38	J/molxK	510.44	Joback Method
cpg	427.79	J/molxK	541.58	Joback Method
cpg	445.27	J/molxK	572.71	Joback Method
cpg	461.88	J/molxK	603.85	Joback Method
cpg	477.63	J/molxK	634.99	Joback Method
cpg	492.57	J/molxK	666.12	Joback Method
cpg	506.72	J/molxK	697.26	Joback Method
dvisc	0.0035337	Paxs	248.69	Joback Method
dvisc	0.0016651	Paxs	292.31	Joback Method

dvisc	0.0009539	Paxs	335.94	Joback Method
dvisc	0.0006212	Paxs	379.56	Joback Method
dvisc	0.0004419	Paxs	423.19	Joback Method
dvisc	0.0003350	Paxs	466.81	Joback Method
dvisc	0.0002663	Paxs	510.44	Joback Method

Sources

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=R40934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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