1,3-Cyclopentadiene, 1-octyl

Inchi: InChI=1S/C13H22/c1-2-3-4-5-6-7-10-13-11-8-9-12-13/h8-9,11H,2-7,10,12H2,1H3
InchiKey: JGLVQJXCFCINBL-UHFFFAOYSA-N
Formula: C13H22
SMILES: CCCCCCCCC1=CC=CC1
Mol. weight [g/mol]: 178.31

Physical Properties

Property code	Value	Unit	Source
gf	153.13	kJ/mol	Joback Method
hf	-126.74	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	46.34	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.623		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1310.00		NIST Webbook
ripol	1507.30		NIST Webbook
tb	520.09	K	Joback Method
tc	708.26	K	Joback Method
tf	265.45	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.99	J/mol×K	520.09	Joback Method
cpg	489.93	J/mol×K	676.90	Joback Method
cpg	475.58	J/mol×K	645.54	Joback Method
cpg	460.44	J/mol×K	614.17	Joback Method
cpg	444.49	J/mol×K	582.81	Joback Method
cpg	427.68	J/mol×K	551.45	Joback Method
cpg	503.54	J/mol×K	708.26	Joback Method
dvisc	0.0002403	Pa×s	520.09	Joback Method

dvisc	0.0003078	Pa×s	477.65	Joback Method
dvisc	0.0004139	Pa×s	435.21	Joback Method
dvisc	0.0005933	Pa×s	392.77	Joback Method
dvisc	0.0009280	Pa×s	350.33	Joback Method
dvisc	0.0016419	Pa×s	307.89	Joback Method
dvisc	0.0034868	Pa×s	265.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R40756&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