

1,3-Cyclopentadiene, 2-octyl

Inchi:	InChI=1S/C13H22/c1-2-3-4-5-6-7-10-13-11-8-9-12-13/h8,11-12H,2-7,9-10H2,1H3
InchiKey:	RBQZNTCEANVLGO-UHFFFAOYSA-N
Formula:	C13H22
SMILES:	CCCCCCCC1=CCC=C1
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
mvol	174.570	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
ripol	1306.00		NIST Webbook
ripol	1497.10		NIST Webbook
tb	520.09	K	Joback Method
tc	708.26	K	Joback Method
tf	265.45	K	Joback Method
vc	0.677	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.99	J/molxK	520.09	Joback Method
cpg	427.68	J/molxK	551.45	Joback Method
cpg	444.49	J/molxK	582.81	Joback Method
cpg	460.44	J/molxK	614.17	Joback Method
cpg	475.58	J/molxK	645.54	Joback Method
cpg	489.93	J/molxK	676.90	Joback Method
cpg	503.54	J/molxK	708.26	Joback Method
dvisc	0.0034868	Paxs	265.45	Joback Method

dvisc	0.0016419	Paxs	307.89	Joback Method
dvisc	0.0009280	Paxs	350.33	Joback Method
dvisc	0.0005933	Paxs	392.77	Joback Method
dvisc	0.0004139	Paxs	435.21	Joback Method
dvisc	0.0003078	Paxs	477.65	Joback Method
dvisc	0.0002403	Paxs	520.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40863&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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