1,3-Cyclopentadiene, 5-heptyl

Inchi: InChI=1S/C12H20/c1-2-3-4-5-6-9-12-10-7-8-11-12/h7-8,10-12H,2-6,9H2,1H3
InchiKey: PBUOSXJXSSMGMT-UHFFFAOYSA-N
Formula: C12H20
SMILES: CCCCCCCC1C=CC=C1
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	146.63	kJ/mol	Joback Method
hf	-114.97	kJ/mol	Joback Method
hfus	23.21	kJ/mol	Joback Method
hvap	43.15	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	4.089		Crippen Method
mcvol	160.480	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1228.00		NIST Webbook
tb	487.56	K	Joback Method
tc	676.50	K	Joback Method
tf	237.42	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.39	J/mol×K	487.56	Joback Method
cpg	379.15	J/mol×K	519.05	Joback Method
cpg	396.02	J/mol×K	550.54	Joback Method
cpg	412.03	J/mol×K	582.03	Joback Method
cpg	427.21	J/mol×K	613.52	Joback Method
cpg	441.60	J/mol×K	645.01	Joback Method
cpg	455.23	J/mol×K	676.50	Joback Method
dvisc	0.0033945	Pa×s	237.42	Joback Method
dvisc	0.0016365	Pa×s	279.11	Joback Method

dvisc	0.0009537	Pa×s	320.80	Joback Method
dvisc	0.0006292	Pa×s	362.49	Joback Method
dvisc	0.0004524	Pa×s	404.18	Joback Method
dvisc	0.0003459	Pa×s	445.87	Joback Method
dvisc	0.0002769	Pa×s	487.56	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=R40916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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