

1,3-Cyclohexadiene, 1-methyl-4-(6-methyl-4-heptenyl)

Inchi:	InChI=1S/C15H24/c1-13(2)7-5-4-6-8-15-11-9-14(3)10-12-15/h5,7,9,11,13H,4,6,8,10,12H
InchiKey:	OTJVAZVIERDNRF-FNORWQNLSA-N
Formula:	C15H24
SMILES:	CC1=CC=C(CCCC=CC(C)C)CC1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	226.02	kJ/mol	Joback Method
hf	-73.71	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	51.20	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.035		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1589.00		NIST Webbook
tb	578.82	K	Joback Method
tc	781.70	K	Joback Method
tf	276.91	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.38	J/molxK	578.82	Joback Method
cpg	513.88	J/molxK	612.63	Joback Method
cpg	532.30	J/molxK	646.45	Joback Method
cpg	549.71	J/molxK	680.26	Joback Method
cpg	566.13	J/molxK	714.07	Joback Method
cpg	581.64	J/molxK	747.89	Joback Method
cpg	596.26	J/molxK	781.70	Joback Method
dvisc	0.0038669	Paxs	276.91	Joback Method
dvisc	0.0014115	Paxs	327.23	Joback Method

dvisc	0.0006740	Paxs	377.55	Joback Method
dvisc	0.0003830	Paxs	427.87	Joback Method
dvisc	0.0002451	Paxs	478.18	Joback Method
dvisc	0.0001708	Paxs	528.50	Joback Method
dvisc	0.0001267	Paxs	578.82	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=R400090&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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