

CYCLOHEXENE, 1,3-DIISOPROPENYL-6-METHYL-

Other names:	Cyclohexene, 1,3-diisopropenyl-6-me
Inchi:	InChI=1S/C13H20/c1-9(2)12-7-6-11(5)13(8-12)10(3)4/h8,11-12H,1,3,6-7H2,2,4-5H3
InchiKey:	SFWPBBHYROOSNZ-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	<chem>C=C(C)C1=CC(C(=C)C)CCC1C</chem>
Mol. weight [g/mol]:	176.30

Physical Properties

Property code	Value	Unit	Source
hfus	17.99	kJ/mol	Joback Method
logp	4.111		Crippen Method
mcpvol	170.270	ml/mol	McGowan Method
tb	496.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.82	J/mol×K	508.98	Joback Method
cpg	411.01	J/mol×K	543.68	Joback Method
cpg	430.13	J/mol×K	578.39	Joback Method
cpg	448.20	J/mol×K	613.09	Joback Method
cpg	465.27	J/mol×K	647.79	Joback Method
cpg	481.37	J/mol×K	682.49	Joback Method
cpg	496.54	J/mol×K	717.20	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151289&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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