

1,3-Cyclohexadiene, 6-methyl

Other names:	1,3-Cyclohexadiene, 6-methyl 5-Methyl-1,3-cyclohexadiene
Inchi:	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-5,7H,6H2,1H3
InchiKey:	ZNKKYYNWFKHNNHZ-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	CC1C=CC=CC1
Mol. weight [g/mol]:	94.16

Physical Properties

Property code	Value	Unit	Source
hfus	8.16	kJ/mol	Joback Method
logp	2.139		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
rinpol	763.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	763.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.80	J/mol×K	377.43	Joback Method
cpg	220.31	J/mol×K	584.34	Joback Method
cpg	210.03	J/mol×K	549.86	Joback Method
cpg	199.13	J/mol×K	515.37	Joback Method
cpg	187.58	J/mol×K	480.89	Joback Method
cpg	175.35	J/mol×K	446.40	Joback Method
cpg	162.43	J/mol×K	411.92	Joback Method
dvisc	0.0005646	Pa×s	277.49	Joback Method
dvisc	0.0002387	Pa×s	377.43	Joback Method
dvisc	0.0003008	Pa×s	344.12	Joback Method
dvisc	0.0003985	Pa×s	310.80	Joback Method
dvisc	0.0035209	Pa×s	177.55	Joback Method
dvisc	0.0008799	Pa×s	244.18	Joback Method
dvisc	0.0015775	Pa×s	210.86	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19656985&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>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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