

CYCLOPROPANE, 1-METHYL-1-(1-METHYLETHENYL)-

Inchi: InChI=1S/C7H12/c1-6(2)7(3)4-5-7/h1,4-5H2,2-3H3

InchiKey: PQMFTBQGLFFXOQ-UHFFFAOYSA-N

Formula: C7H12

SMILES: C=C(C)C1(C)CC1

Mol. weight [g/mol]: 96.17

Physical Properties

Property code	Value	Unit	Source
hfus	3.13	kJ/mol	Joback Method
ie	9.03	eV	NIST Webbook
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
tb	357.42	K	Cheméo Relay (1.0)
tf	201.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.70	J/mol×K	363.10	Joback Method
cpg	178.02	J/mol×K	395.53	Joback Method
cpg	191.17	J/mol×K	427.96	Joback Method
cpg	203.25	J/mol×K	460.40	Joback Method
cpg	214.37	J/mol×K	492.83	Joback Method
cpg	224.62	J/mol×K	525.26	Joback Method
cpg	234.09	J/mol×K	557.69	Joback Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3422079&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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