

1,3-DIMETHYLCYCLOPENTENE

Inchi:	InChI=1S/C7H12/c1-6-3-4-7(2)5-6/h5-6H,3-4H2,1-2H3
InchiKey:	QIIAONVJAUZQQR-LURJTMIESA-N
Formula:	C7H12
SMILES:	CC1=CC(C)CC1
Mol. weight [g/mol]:	96.17

Physical Properties

Property code	Value	Unit	Source
gf	64.94	kJ/mol	Joback Method
hf	-81.02	kJ/mol	Joback Method
hfus	8.65	kJ/mol	Joback Method
hvap	32.39	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	378.98	K	Joback Method
tc	576.72	K	Joback Method
tf	192.83	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.57	J/molxK	378.98	Joback Method
cpg	225.59	J/molxK	543.77	Joback Method
cpg	214.58	J/molxK	510.81	Joback Method
cpg	202.99	J/molxK	477.85	Joback Method
cpg	190.80	J/molxK	444.89	Joback Method
cpg	178.00	J/molxK	411.94	Joback Method
cpg	236.05	J/molxK	576.72	Joback Method
dvisc	0.0002552	Paxs	378.98	Joback Method
dvisc	0.0003032	Paxs	347.96	Joback Method
dvisc	0.0003727	Paxs	316.93	Joback Method

dvisc	0.0004791	Paxs	285.90	Joback Method
dvisc	0.0006547	Paxs	254.88	Joback Method
dvisc	0.0009756	Paxs	223.85	Joback Method
dvisc	0.0016528	Paxs	192.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=620
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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