

# Heptafulvene

<b>Inchi:</b>	InChI=1S/C8H8/c1-8-6-4-2-3-5-7-8/h2-7H,1H2
<b>InchiKey:</b>	GGKMDDDYCSVHMU-UHFFFAOYSA-N
<b>Formula:</b>	C8H8
<b>SMILES:</b>	C=C1C=CC=CC=C1
<b>Mol. weight [g/mol]:</b>	104.15
<b>CAS:</b>	539-79-7

## Physical Properties

Property code	Value	Unit	Source
gf	179.50	kJ/mol	Joback Method
hf	117.63	kJ/mol	Joback Method
hfus	7.65	kJ/mol	Joback Method
hvap	35.35	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.225		Crippen Method
mcvol	95.520	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	407.57	K	Joback Method
tc	626.47	K	Joback Method
tf	203.98	K	Joback Method
vc	0.351	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.68	J/molxK	407.57	Joback Method
cpg	172.17	J/molxK	444.05	Joback Method
cpg	183.95	J/molxK	480.54	Joback Method
cpg	195.03	J/molxK	517.02	Joback Method
cpg	205.43	J/molxK	553.50	Joback Method
cpg	215.18	J/molxK	589.98	Joback Method
cpg	224.30	J/molxK	626.47	Joback Method
dvisc	0.0042265	Paxs	203.98	Joback Method
dvisc	0.0018145	Paxs	237.91	Joback Method

dvisc	0.0009620	Paxs	271.84	Joback Method
dvisc	0.0005872	Paxs	305.77	Joback Method
dvisc	0.0003956	Paxs	339.71	Joback Method
dvisc	0.0002863	Paxs	373.64	Joback Method
dvisc	0.0002187	Paxs	407.57	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C539797&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C539797&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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