

3-Methoxy-1-methyl-1,3-cyclohexadiene

Inchi:	InChI=1S/C8H12O/c1-7-4-3-5-8(6-7)9-2/h5-6H,3-4H2,1-2H3
InchiKey:	IGWOPMYDPJKFJT-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	COC1=CCCC(C)=C1
Mol. weight [g/mol]:	124.18
CAS:	98677-97-5

Physical Properties

Property code	Value	Unit	Source
gf	-15.70	kJ/mol	Joback Method
hf	-173.39	kJ/mol	Joback Method
hfus	10.09	kJ/mol	Joback Method
hvap	38.46	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.257		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	437.36	K	Joback Method
tc	645.03	K	Joback Method
tf	240.33	K	Joback Method
vc	0.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.23	J/molxK	437.36	Joback Method
cpg	226.45	J/molxK	471.97	Joback Method
cpg	239.09	J/molxK	506.58	Joback Method
cpg	251.16	J/molxK	541.19	Joback Method
cpg	262.67	J/molxK	575.80	Joback Method
cpg	273.62	J/molxK	610.42	Joback Method
cpg	284.02	J/molxK	645.03	Joback Method
dvisc	0.0021942	Paxs	240.33	Joback Method
dvisc	0.0011661	Paxs	273.17	Joback Method

dvisc	0.0007098	Paxs	306.01	Joback Method
dvisc	0.0004757	Paxs	338.85	Joback Method
dvisc	0.0003422	Paxs	371.68	Joback Method
dvisc	0.0002596	Paxs	404.52	Joback Method
dvisc	0.0002054	Paxs	437.36	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98677975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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