1-Methoxy-1,3-cyclohexadiene

Other names:	1,3-Cyclohexadiene, 1-methoxy-
	1-methoxycyclohexa-1,3-diene
Inchi:	InChI=1S/C7H10O/c1-8-7-5-3-2-4-6-7/h2-3,5H,4,6H2,1H3
InchiKey:	LNRUJSUKKBJFOM-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	COC1=CC=CCC1
Mol. weight [g/mol]:	110.15
CAS:	2161-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-14.49	kJ/mol	Joback Method
hf	-141.28	kJ/mol	Joback Method
hfus	7.89	kJ/mol	Joback Method
hvap	35.57	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.867		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	904.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1250.00		NIST Webbook
tb	409.50	K	Joback Method
tc	618.03	K	Joback Method
tf	216.54	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.00	J/mol×K	409.50	Joback Method
cpg	185.38	J/mol×K	444.25	Joback Method

cpg	197.19	J/mol×K	479.01	Joback Method
cpg	208.43	J/mol×K	513.76	Joback Method
cpg	219.11	J/mol×K	548.52	Joback Method
cpg	229.25	J/mol×K	583.27	Joback Method
cpg	238.85	J/mol×K	618.03	Joback Method
dvisc	0.0031599	Pa×s	216.54	Joback Method
dvisc	0.0015242	Pa×s	248.70	Joback Method
dvisc	0.0008688	Pa×s	280.86	Joback Method
dvisc	0.0005559	Pa×s	313.02	Joback Method
dvisc	0.0003865	Pa×s	345.18	Joback Method
dvisc	0.0002859	Pa×s	377.34	Joback Method
dvisc	0.0002218	Pa×s	409.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	313.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2161902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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