

1-Methoxy-1,4-cyclohexadiene

Other names:	1,4-Cyclohexadiene, 1-methoxy- 1-methoxycyclohexa-1,4-diene
Inchi:	InChI=1S/C7H10O/c1-8-7-5-3-2-4-6-7/h2-3,6H,4-5H2,1H3
InchiKey:	RGXIXVNKYUAKHS-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	COC1=CCC=CC1
Mol. weight [g/mol]:	110.15
CAS:	2886-59-1

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
mvol	95.900	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	939.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	939.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1268.00		NIST Webbook
tb	422.20	K	NIST Webbook
tc	618.03	K	Joback Method
tf	216.54	K	Joback Method
vc	0.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.00	J/molxK	409.50	Joback Method

cpg	229.25	J/molxK	583.27	Joback Method
cpg	219.11	J/molxK	548.52	Joback Method
cpg	208.43	J/molxK	513.76	Joback Method
cpg	197.19	J/molxK	479.01	Joback Method
cpg	185.38	J/molxK	444.25	Joback Method
cpg	238.85	J/molxK	618.03	Joback Method
dvisc	0.0002218	Paxs	409.50	Joback Method
dvisc	0.0002859	Paxs	377.34	Joback Method
dvisc	0.0003865	Paxs	345.18	Joback Method
dvisc	0.0005559	Paxs	313.02	Joback Method
dvisc	0.0008688	Paxs	280.86	Joback Method
dvisc	0.0015242	Paxs	248.70	Joback Method
dvisc	0.0031599	Paxs	216.54	Joback Method

Sources

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=C2886591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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