3-Methoxy-1,5-dimethyl-1,3-cyclohexadiene

Inchi: InChI=1S/C9H14O/c1-7-4-8(2)6-9(5-7)10-3/h5-7H,4H2,1-3H3
InchiKey: SNEXTYOVZVMOCT-UHFFFAOYSA-N
Formula: C9H14O
SMILES: COC1=CC(C)CC(C)=C1
Mol. weight [g/mol]: 138.21
CAS: 98677-98-6

Physical Properties

Property code	Value	Unit	Source
gf	-14.99	kJ/mol	Joback Method
hf	-214.37	kJ/mol	Joback Method
hfus	13.75	kJ/mol	Joback Method
hvap	40.38	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.503		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	455.57	K	Joback Method
tc	660.32	K	Joback Method
tf	247.36	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.17	J/mol×K	455.57	Joback Method
cpg	269.90	J/mol×K	489.69	Joback Method
cpg	284.03	J/mol×K	523.82	Joback Method
cpg	297.54	J/mol×K	557.94	Joback Method
cpg	310.45	J/mol×K	592.07	Joback Method
cpg	322.75	J/mol×K	626.19	Joback Method
cpg	334.45	J/mol×K	660.32	Joback Method
dvisc	0.0015726	Pa×s	247.36	Joback Method
dvisc	0.0009053	Pa×s	282.06	Joback Method

dvisc	0.0005882	Pa×s	316.76	Joback Method
dvisc	0.0004162	Pa×s	351.47	Joback Method
dvisc	0.0003133	Pa×s	386.17	Joback Method
dvisc	0.0002472	Pa×s	420.87	Joback Method
dvisc	0.0002022	Pa×s	455.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98677986&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

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