2-Methoxy-1,3-cycloheptadiene

Inchi: InChI=1S/C8H12O/c1-9-8-6-4-2-3-5-7-8/h4,6-7H,2-3,5H2,1H3
InchiKey: JYVRGXIYJXJIBY-UHFFFAOYSA-N
Formula: C8H12O
SMILES: COC1=CCCCC=C1
Mol. weight [g/mol]: 124.18
CAS: 98677-95-3

Physical Properties

Property code	Value	Unit	Source
gf	-18.17	kJ/mol	Joback Method
hf	-168.08	kJ/mol	Joback Method
hfus	8.38	kJ/mol	Joback Method
hvap	37.97	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.257		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	436.65	K	Joback Method
tc	651.38	K	Joback Method
tf	224.29	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.96	J/mol×K	436.65	Joback Method
cpg	225.63	J/mol×K	472.44	Joback Method
cpg	239.62	J/mol×K	508.23	Joback Method
cpg	252.92	J/mol×K	544.01	Joback Method
cpg	265.55	J/mol×K	579.80	Joback Method
cpg	277.51	J/mol×K	615.59	Joback Method
cpg	288.80	J/mol×K	651.38	Joback Method
dvisc	0.0052003	Pa×s	224.29	Joback Method
dvisc	0.0020544	Pa×s	259.68	Joback Method

dvisc	0.0010141	Pa×s	295.08	Joback Method
dvisc	0.0005824	Pa×s	330.47	Joback Method
dvisc	0.0003723	Pa×s	365.86	Joback Method
dvisc	0.0002575	Pa×s	401.26	Joback Method
dvisc	0.0001891	Pa×s	436.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98677953&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