Ether, 2,4,6-cycloheptatrien-1-yl methyl

Other names:	1,3,5-Cycloheptatriene, 7-methoxy- 7-Methoxy-1,3,5-cycloheptatriene 7-Methoxycycloheptatriene 7-Methoxycyclohepta-1,3,5-triene
Inchi:	InChI=1S/C8H10O/c1-9-8-6-4-2-3-5-7-8/h2-8H,1H3
InchiKey:	RUJLQZXBIZHGNF-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	COC1C=CC=CC=C1
Mol. weight [g/mol]:	122.16
CAS:	1714-38-1

Physical Properties

Property code	Value	Unit	Source
gf	13.71	kJ/mol	Joback Method
hf	-119.17	kJ/mol	Joback Method
hfus	11.06	kJ/mol	Joback Method
hvap	37.29	kJ/mol	Joback Method
ie	7.23	eV	NIST Webbook
log10ws	-1.83		Crippen Method
logp	1.684		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	426.16	K	Joback Method
tc	641.28	K	Joback Method
tf	208.29	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.41	J/mol×K	426.16	Joback Method
cpg	210.54	J/mol×K	462.01	Joback Method
cpg	223.99	J/mol×K	497.87	Joback Method
cpg	236.75	J/mol×K	533.72	Joback Method

cpg	248.85	J/mol×K	569.57	Joback Method
cpg	260.27	J/mol×K	605.42	Joback Method
cpg	271.03	J/mol×K	641.28	Joback Method
dvisc	0.0039749	Pa×s	208.29	Joback Method
dvisc	0.0016470	Pa×s	244.60	Joback Method
dvisc	0.0008570	Pa×s	280.91	Joback Method
dvisc	0.0005179	Pa×s	317.23	Joback Method
dvisc	0.0003471	Pa×s	353.54	Joback Method
dvisc	0.0002506	Pa×s	389.85	Joback Method
dvisc	0.0001913	Pa×s	426.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1714381&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
ie: Ionization energy
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

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