

7-Methoxycycloheptatriene

Other names:

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

1,3,5-Cycloheptatriene, 7-methoxy-
7-Methoxy-1,3,5-cycloheptatriene
7-Methoxycycloheptatriene
7-Methoxycyclohepta-1,3,5-triene

InChI=1S/C8H10O/c1-9-8-6-4-2-3-5-7-8/h2-8H,1H3

RUJLQZXBIZHGNF-UHFFFAOYSA-N

C8H10O

COC1C=CC=CC=C1

122.17

Physical Properties

Property code	Value	Unit	Source
hfus	11.06	kJ/mol	Joback Method
ie	7.23	eV	NIST Webbook
logp	1.684		Crippen Method
mcvol	105.690	ml/mol	McGowan 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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1714381&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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