3-Cyclohexene-1-carboxylic acid, methyl ester

Other names:	Methyl 1,2,3,6-tetrahydrobenzoate
	Methyl 3-cyclohexene-1-carboxylate
	Methyl 3-cyclohexenecarboxylate
	Methyl 4-cyclohexenecarboxylate
	1-Carbomethoxy-3-cyclohexene
	1,3-Butadiene-methyl acrylate adduct
	Methyl ester of 3-cyclohexene-1-carboxylic acid
	methyl cyclohex-3-enecarboxylate
Inchi:	InChI=1S/C8H12O2/c1-10-8(9)7-5-3-2-4-6-7/h2-3,7H,4-6H2,1H3
InchiKey:	IPUNVLFESXFVFH-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	COC(=O)C1CC=CCC1
Mol. weight [g/mol]:	140.18
CAS:	6493-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-163.03	kJ/mol	Joback Method
hf	-341.15	kJ/mol	Joback Method
hfus	12.32	kJ/mol	Joback Method
hvap	43.28	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.516		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
ripol	1446.60		NIST Webbook
ripol	1446.60		NIST Webbook
tb	477.44	K	Joback Method
tc	691.16	K	Joback Method
tf	260.22	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.26	J/mol×K	477.44	Joback Method
cpg	262.12	J/mol×K	513.06	Joback Method
cpg	276.22	J/mol×K	548.68	Joback Method
cpg	289.57	J/mol×K	584.30	Joback Method
cpg	302.19	J/mol×K	619.92	Joback Method
cpg	314.08	J/mol×K	655.54	Joback Method
cpg	325.25	J/mol×K	691.16	Joback Method
dvisc	0.0035229	Pa×s	260.22	Joback Method
dvisc	0.0017750	Pa×s	296.42	Joback Method
dvisc	0.0010382	Pa×s	332.63	Joback Method
dvisc	0.0006747	Pa×s	368.83	Joback Method
dvisc	0.0004736	Pa×s	405.03	Joback Method
dvisc	0.0003523	Pa×s	441.24	Joback Method
dvisc	0.0002741	Pa×s	477.44	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6493772&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume