Methyl 1-cyclohexene-1-carboxylate

Other names:	1-Cyclohexene-1-carboxylic acid, methyl ester
	Methyl 1-Cyclohexenecarboxylate
	methyl cyclohex-1-ene-1-carboxylate
Inchi:	InChI=1S/C8H12O2/c1-10-8(9)7-5-3-2-4-6-7/h5H,2-4,6H2,1H3
InchiKey:	KXPWRCPEMHIZGU-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	COC(=O)C1=CCCCC1
Mol. weight [g/mol]:	140.18
CAS:	18448-47-0

Physical Properties

Property code	Value	Unit	Source
gf	-164.95	kJ/mol	Joback Method
hf	-332.28	kJ/mol	Joback Method
hfus	10.86	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.660		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	464.20	K	NIST Webbook
tc	702.33	K	Joback Method
tf	276.98	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.79	J/mol×K	487.09	Joback Method
cpg	260.87	J/mol×K	522.96	Joback Method
cpg	274.23	J/mol×K	558.84	Joback Method
cpg	286.88	J/mol×K	594.71	Joback Method
cpg	298.83	J/mol×K	630.58	Joback Method
cpg	310.09	J/mol×K	666.46	Joback Method

cpg	320.67	J/mol×K	702.33	Joback Method
dvisc	0.0032998	Pa×s	276.98	Joback Method
dvisc	0.0016861	Pa×s	312.00	Joback Method
dvisc	0.0009866	Pa×s	347.02	Joback Method
dvisc	0.0006369	Pa×s	382.03	Joback Method
dvisc	0.0004425	Pa×s	417.05	Joback Method
dvisc	0.0003253	Pa×s	452.07	Joback Method
dvisc	0.0002499	Pa×s	487.09	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18448470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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