3-Cyclohexene-1-carboxylic acid, 4-methyl-, methyl ester

Other names: Methyl 4-methyl-3-cyclohexene-1-carboxylate
4-Methoxycarbonyl-1-methylcyclohexene
1-carbomethoxy-4-methylcyclohex-3-ene

Inchi: InChI=1S/C9H14O2/c1-7-3-5-8(6-4-7)9(10)11-2/h3,8H,4-6H2,1-2H3

InchiKey: JNDBPUPULVCVFC-UHFFFAOYSA-N

Formula: C9H14O2

SMILES: COC(=O)C1CC=C(C)CC1

Mol. weight [g/mol]: 154.21

CAS: 6493-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-164.24	kJ/mol	Joback Method
hf	-373.26	kJ/mol	Joback Method
hfus	14.52	kJ/mol	Joback Method
hvap	46.17	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.906		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
ripol	1586.90		NIST Webbook
ripol	1557.70		NIST Webbook
ripol	1557.70		NIST Webbook
tb	505.30	K	Joback Method
tc	717.03	K	Joback Method
tf	284.01	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.84	J/mol×K	505.30	Joback Method
cpg	361.73	J/mol×K	681.74	Joback Method
cpg	349.24	J/mol×K	646.45	Joback Method

cpg	336.01	J/mol×K	611.16	Joback Method
cpg	322.04	J/mol×K	575.88	Joback Method
cpg	307.31	J/mol×K	540.59	Joback Method
cpg	373.48	J/mol×K	717.03	Joback Method
dvisc	0.0002497	Pa×s	505.30	Joback Method
dvisc	0.0003156	Pa×s	468.42	Joback Method
dvisc	0.0004152	Pa×s	431.54	Joback Method
dvisc	0.0005749	Pa×s	394.65	Joback Method
dvisc	0.0008515	Pa×s	357.77	Joback Method
dvisc	0.0013801	Pa×s	320.89	Joback Method
dvisc	0.0025360	Pa×s	284.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6493794&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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