Cyclohexanecarboxylic acid, methyl ester

Other names:	Hexahydrobenzoic acid methyl ester
	Methyl cyclohexanecarboxylate
	Methyl cyclohexanoate
	Methyl cyclohexylcarboxylate
	Methyl ester of cyclohexanecarboxylic acid
	c-C6H11COOCH3
Inchi:	InChI=1S/C8H14O2/c1-10-8(9)7-5-3-2-4-6-7/h7H,2-6H2,1H3
InchiKey:	ZQWPRMPSCMSAJU-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	COC(=O)C1CCCCC1
Mol. weight [g/mol]:	142.20
CAS:	4630-82-4

Physical Properties

Property code	Value	Unit	Source
affp	846.20	kJ/mol	NIST Webbook
basg	815.30	kJ/mol	NIST Webbook
gf	-192.99	kJ/mol	Joback Method
hf	-398.93	kJ/mol	Joback Method
hfus	11.10	kJ/mol	Joback Method
hvap	42.99	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.740		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	1011.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1005.17		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1009.57		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.17		NIST Webbook

ripol	1385.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1385.00		NIST Webbook
tb	456.20	K	NIST Webbook
tb	456.20 ± 1.00	K	NIST Webbook
tc	689.84	K	Joback Method
tf	259.46	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.26	J/mol×K	478.28	Joback Method
cpg	279.37	J/mol×K	513.54	Joback Method
cpg	294.69	J/mol×K	548.80	Joback Method
cpg	309.24	J/mol×K	584.06	Joback Method
cpg	323.01	J/mol×K	619.32	Joback Method
cpg	336.02	J/mol×K	654.58	Joback Method
cpg	348.27	J/mol×K	689.84	Joback Method
dvisc	0.0043366	Pa×s	259.46	Joback Method
dvisc	0.0020707	Pa×s	295.93	Joback Method
dvisc	0.0011629	Pa×s	332.40	Joback Method
dvisc	0.0007320	Pa×s	368.87	Joback Method
dvisc	0.0005008	Pa×s	405.34	Joback Method
dvisc	0.0003648	Pa×s	441.81	Joback Method
dvisc	0.0002788	Pa×s	478.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4630824&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

affp:	Proton affinity
basg:	Gas basicity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume