

Methyl cyclohexanecarboxylate, 4-(1,1-dimethylethyl), # 1

Inchi: InChI=1S/C12H22O2/c1-12(2,3)10-7-5-9(6-8-10)11(13)14-4/h9-10H,5-8H2,1-4H3
InchiKey: BWJSSYBIZVGKBG-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: COC(=O)C1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-164.18	kJ/mol	Joback Method
hf	-510.58	kJ/mol	Joback Method
hfus	15.12	kJ/mol	Joback Method
hvap	50.29	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	3.012		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1639.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1639.00		NIST Webbook
tb	561.90	K	Joback Method
tc	773.24	K	Joback Method
tf	302.72	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.11	J/mol×K	561.90	Joback Method
cpg	478.84	J/mol×K	597.12	Joback Method

cpg	498.39	J/mol×K	632.35	Joback Method
cpg	516.77	J/mol×K	667.57	Joback Method
cpg	534.02	J/mol×K	702.79	Joback Method
cpg	550.18	J/mol×K	738.01	Joback Method
cpg	565.28	J/mol×K	773.24	Joback Method
dvisc	0.0039043	Pa×s	302.72	Joback Method
dvisc	0.0017642	Pa×s	345.92	Joback Method
dvisc	0.0009509	Pa×s	389.11	Joback Method
dvisc	0.0005799	Pa×s	432.31	Joback Method
dvisc	0.0003869	Pa×s	475.51	Joback Method
dvisc	0.0002762	Pa×s	518.70	Joback Method
dvisc	0.0002076	Pa×s	561.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R97773&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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