

Methyl cyclopentanecarboxylate

Other names:	Cyclopentanecarboxylic acid, methyl ester
Inchi:	InChI=1S/C7H12O2/c1-9-7(8)6-4-2-3-5-6/h6H,2-5H2,1H3
InchiKey:	IIHIJFSXPDTNO-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	COC(=O)C1CCCC1
Mol. weight [g/mol]:	128.17
CAS:	4630-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-189.31	kJ/mol	Joback Method
hf	-372.13	kJ/mol	Joback Method
hfus	10.61	kJ/mol	Joback Method
hvap	40.59	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.350		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	898.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	902.00		NIST Webbook
tb	451.13	K	Joback Method
tc	657.44	K	Joback Method
tf	251.71	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.09	J/molxK	451.13	Joback Method
cpg	235.14	J/molxK	485.51	Joback Method
cpg	248.51	J/molxK	519.90	Joback Method
cpg	261.22	J/molxK	554.28	Joback Method
cpg	273.28	J/molxK	588.67	Joback Method

cpg	284.70	J/molxK	623.05	Joback Method
cpg	295.49	J/molxK	657.44	Joback Method
dvisc	0.0030776	Paxs	251.71	Joback Method
dvisc	0.0017254	Paxs	284.95	Joback Method
dvisc	0.0010917	Paxs	318.18	Joback Method
dvisc	0.0007532	Paxs	351.42	Joback Method
dvisc	0.0005540	Paxs	384.66	Joback Method
dvisc	0.0004280	Paxs	417.89	Joback Method
dvisc	0.0003434	Paxs	451.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4630802&Units=SI

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

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