Cyclopentanecarboxylic acid, 1-methyl-

Inchi: InChI=1S/C7H12O2/c1-7(6(8)9)4-2-3-5-7/h2-5H2,1H3,(H,8,9)
InchiKey: MNIBBVOEXUQHFF-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: CC1(C(=O)O)CCCC1
Mol. weight [g/mol]: 128.17
CAS: 5217-05-0

Physical Properties

Property code	Value	Unit	Source
gf	-226.62	kJ/mol	Joback Method
hf	-376.90	kJ/mol	Joback Method
hfus	7.21	kJ/mol	Joback Method
hvap	53.71	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.651		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
tb	492.20	K	NIST Webbook
tc	724.40	K	Joback Method
tf	314.20	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.83	J/mol×K	521.13	Joback Method
cpg	261.61	J/mol×K	555.01	Joback Method
cpg	272.61	J/mol×K	588.89	Joback Method
cpg	282.90	J/mol×K	622.76	Joback Method
cpg	292.60	J/mol×K	656.64	Joback Method
cpg	301.79	J/mol×K	690.52	Joback Method
cpg	310.57	J/mol×K	724.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.70	K	2.10	NIST Webbook

Sources

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=C5217050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume