2-Cyclopentene-1-carboxylic acid, 1-methyl-

Inchi: InChI=1S/C7H10O2/c1-7(6(8)9)4-2-3-5-7/h2,4H,3,5H2,1H3,(H,8,9)
InchiKey: HGSACGMRDLYHMZ-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1(C(=O)O)C=CCC1
Mol. weight [g/mol]: 126.15
CAS: 68317-77-1

Physical Properties

Property code	Value	Unit	Source
gf	-196.66	kJ/mol	Joback Method
hf	-319.12	kJ/mol	Joback Method
hfus	8.43	kJ/mol	Joback Method
hvap	54.00	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.427		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
rinpol	1085.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1085.00		NIST Webbook
tb	520.29	K	Joback Method
tc	725.51	K	Joback Method
tf	314.96	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.20	J/mol×K	520.29	Joback Method
cpg	242.80	J/mol×K	554.49	Joback Method
cpg	252.63	J/mol×K	588.70	Joback Method
cpg	261.79	J/mol×K	622.90	Joback Method
cpg	270.39	J/mol×K	657.10	Joback Method
cpg	278.53	J/mol×K	691.30	Joback Method

cpg	286.30	J/mol×K	725.51	Joback Method

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=C68317771&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume