1-Methylcyclopropanecarboxylic acid

Other names: 1-Methylcyclopropane-1-carboxylic acid
Cyclopropanecarboxylic acid, 1-methyl-
Inchi: InChI=1S/C5H8O2/c1-5(2-3-5)4(6)7/h2-3H2,1H3,(H,6,7)
InchiKey: DIZKLZKLNKQFGB-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: CC1(C(=O)O)CC1
Mol. weight [g/mol]: 100.12
CAS: 6914-76-7

Physical Properties

Property code	Value	Unit	Source
gf	-219.26	kJ/mol	Joback Method
hf	-323.30	kJ/mol	Joback Method
hfus	6.23	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.871		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
tb	457.20	K	NIST Webbook
tc	660.75	K	Joback Method
tf	303.90 ± 4.00	K	NIST Webbook
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.51	J/mol×K	466.83	Joback Method
cpg	176.98	J/mol×K	499.15	Joback Method
cpg	184.72	J/mol×K	531.47	Joback Method
cpg	191.84	J/mol×K	563.79	Joback Method
cpg	198.41	J/mol×K	596.11	Joback Method
cpg	204.54	J/mol×K	628.43	Joback Method
cpg	210.31	J/mol×K	660.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6914767&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume