

2-Methylcyclopropanecarboxylic acid

Other names:	Cyclopropanecarboxylic acid, 2-methyl-
Inchi:	InChI=1S/C5H8O2/c1-3-2-4(3)5(6)7/h3-4H,2H2,1H3,(H,6,7)
InchiKey:	AYEGPMGNMOIHDL-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC1CC1C(=O)O
Mol. weight [g/mol]:	100.12
CAS:	29555-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-221.48	kJ/mol	Joback Method
hf	-358.88	kJ/mol	Joback Method
hfus	13.60	kJ/mol	Joback Method
hvap	49.75	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.727		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	461.92	K	Joback Method
tc	647.68	K	Joback Method
tf	270.56	K	Joback Method
vc	0.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.33	J/molxK	461.92	Joback Method
cpg	178.18	J/molxK	492.88	Joback Method
cpg	186.56	J/molxK	523.84	Joback Method
cpg	194.48	J/molxK	554.80	Joback Method
cpg	201.98	J/molxK	585.76	Joback Method
cpg	209.06	J/molxK	616.72	Joback Method
cpg	215.76	J/molxK	647.68	Joback Method
dvisc	0.0092179	Paxs	270.56	Joback Method

dvisc	0.0042550	Paxs	302.45	Joback Method
dvisc	0.0022763	Paxs	334.35	Joback Method
dvisc	0.0013579	Paxs	366.24	Joback Method
dvisc	0.0008799	Paxs	398.13	Joback Method
dvisc	0.0006081	Paxs	430.03	Joback Method
dvisc	0.0004422	Paxs	461.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.70	K	99.30	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=C29555020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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