

Cyclopropanecarboxylic acid, 2,3-dimethyl-, methyl ester

Inchi:	InChI=1S/C7H12O2/c1-4-5(2)6(4)7(8)9-3/h4-6H,1-3H3
InchiKey:	KQVXZDVLCHFJMZ-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	COC(=O)C1C(C)C1C
Mol. weight [g/mol]:	128.17
CAS:	72258-11-8

Physical Properties

Property code	Value	Unit	Source
gf	-180.53	kJ/mol	Joback Method
hf	-400.49	kJ/mol	Joback Method
hfus	16.95	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	1.061		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	433.25	K	Joback Method
tc	623.25	K	Joback Method
tf	250.27	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.67	J/molxK	433.25	Joback Method
cpg	237.46	J/molxK	464.92	Joback Method
cpg	249.73	J/molxK	496.58	Joback Method
cpg	261.47	J/molxK	528.25	Joback Method
cpg	272.70	J/molxK	559.92	Joback Method
cpg	283.43	J/molxK	591.58	Joback Method
cpg	293.66	J/molxK	623.25	Joback Method
dvisc	0.0007590	Paxs	250.27	Joback Method
dvisc	0.0006586	Paxs	280.77	Joback Method

dvisc	0.0005877	Paxs	311.26	Joback Method
dvisc	0.0005352	Paxs	341.76	Joback Method
dvisc	0.0004949	Paxs	372.26	Joback Method
dvisc	0.0004631	Paxs	402.75	Joback Method
dvisc	0.0004374	Paxs	433.25	Joback Method

Sources

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=C72258118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/46-310-6/Cyclopropanecarboxylic-acid-2-3-dimethyl-methyl-ester.pdf>

Generated by Cheméo on 2024-04-27 04:49:43.477842586 +0000 UTC m=+16482632.398419899.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.