Cyclopropanecarboxylic acid, methyl ester

Other names: Methyl cyclopropylcarboxylate
methyl cyclopropanecarboxylate
Inchi: InChI=1S/C5H8O2/c1-7-5(6)4-2-3-4/h4H,2-3H2,1H3
InchiKey: PKAHQJNJPDVTDP-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: COC(=O)C1CC1
Mol. weight [g/mol]: 100.12
CAS: 2868-37-3

Physical Properties

Property code	Value	Unit	Source
affp	842.10	kJ/mol	NIST Webbook
basg	811.20	kJ/mol	NIST Webbook
chl	-2764.90 ± 1.50	kJ/mol	NIST Webbook
gf	-181.95	kJ/mol	Joback Method
hf	-304.70 ± 1.50	kJ/mol	NIST Webbook
hfl	-346.00 ± 1.50	kJ/mol	NIST Webbook
hfus	9.63	kJ/mol	Joback Method
hvap	41.30 ± 0.10	kJ/mol	NIST Webbook
hvap	41.27 ± 0.06	kJ/mol	NIST Webbook
hvap	41.30	kJ/mol	NIST Webbook
log10ws	-0.43		Crippen Method
logp	0.569		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	388.00	K	NIST Webbook
tc	591.10	K	Joback Method
tf	236.21	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.56	J/mol×K	396.83	Joback Method

cpg	156.32	J/mol×K	429.21	Joback Method
cpg	165.61	J/mol×K	461.59	Joback Method
cpg	174.42	J/mol×K	493.97	Joback Method
cpg	182.79	J/mol×K	526.34	Joback Method
cpg	190.72	J/mol×K	558.72	Joback Method
cpg	198.24	J/mol×K	591.10	Joback Method
dvisc	0.0009247	Pa×s	262.98	Joback Method
dvisc	0.0012151	Pa×s	236.21	Joback Method
dvisc	0.0007401	Pa×s	289.75	Joback Method
dvisc	0.0006152	Pa×s	316.52	Joback Method
dvisc	0.0005262	Pa×s	343.29	Joback Method
dvisc	0.0004605	Pa×s	370.06	Joback Method
dvisc	0.0004102	Pa×s	396.83	Joback Method
hvapt	35.25	kJ/mol	388.00	NIST Webbook
hvapt	42.60 ± 0.40	kJ/mol	293.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	102.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2868373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibria on Three Binary Systems: Methyl Cyclopropanecarboxalate + Water; Dimethyl Sulfide + Water; and Dimethyl Disulfide + Water:	https://www.doi.org/10.1021/je050326t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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