1-Carboxycyclopropane-2-acetic acid (Z), dimethyl ester

Other names: Methyl 2-(2-methoxy-2-oxoethyl)cyclopropanecarboxylate, (Z)-
2-Methoxycarbonylmethyl-cyclopropanecarboxylic acid methyl ester, Z

Inchi: InChI=1S/C8H12O4/c1-11-7(9)4-5-3-6(5)8(10)12-2/h5-6H,3-4H2,1-2H3/t5-,6-/m1/s1

InchiKey: UXTUIDNFTDLRIX-PHDIDXHHSA-N

Formula: C8H12O4

SMILES: COC(=O)CC1CC1C(=O)OC

Mol. weight [g/mol]: 172.18

CAS: 77462-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-398.32	kJ/mol	Joback Method
hf	-645.59	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	0.359		Crippen Method
mcvol	127.600	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1175.00		NIST Webbook
tb	537.09	K	Joback Method
tc	733.84	K	Joback Method
tf	337.94	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.99	J/mol×K	537.09	Joback Method
cpg	321.47	J/mol×K	569.88	Joback Method
cpg	333.36	J/mol×K	602.67	Joback Method
cpg	344.67	J/mol×K	635.46	Joback Method
cpg	355.42	J/mol×K	668.25	Joback Method

cpg	365.61	J/mol×K	701.05	Joback Method
cpg	375.24	J/mol×K	733.84	Joback Method
dvisc	0.0016772	Pa×s	337.94	Joback Method
dvisc	0.0012748	Pa×s	371.13	Joback Method
dvisc	0.0010135	Pa×s	404.32	Joback Method
dvisc	0.0008344	Pa×s	437.51	Joback Method
dvisc	0.0007060	Pa×s	470.71	Joback Method
dvisc	0.0006106	Pa×s	503.90	Joback Method
dvisc	0.0005377	Pa×s	537.09	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=C77462534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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