

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

Other names:

Methyl 2-(2-methoxy-2-oxoethyl)cyclopropanecarboxylate, trans-2-Methoxycarbonylmethyl-cyclopropanecarboxylic acid methyl ester, E

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+/m0/s1

InchiKey:

UXTUIDNFTDLRIX-RITPCOANSA-N

Formula:

C8H12O4

SMILES:

COC(=O)C[C@@H]1C[C@H]1C(=O)OC

Mol. weight [g/mol]:

172.18

Physical Properties

Property code	Value	Unit	Source
hfus	21.26	kJ/mol	Joback Method
logp	0.359		Crippen Method
mcvol	127.600	ml/mol	McGowan Method
rinpol	1190.00		NIST Webbook
tb	483.18	K	Cheméo Relay (1.0)

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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77462545&Units=SI
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
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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