1,1-Cyclopropanedicarboxylic acid dimethyl ester

Inchi: InChI=1S/C7H10O4/c1-10-5(8)7(3-4-7)6(9)11-2/h3-4H2,1-2H3
InchiKey: PWLLZZMFFZUSOG-UHFFFAOYSA-N
Formula: C7H10O4
SMILES: COC(=O)C1(C(=O)OC)CC1
Mol. weight [g/mol]: 158.15
CAS: 6914-71-2

Physical Properties

Property code	Value	Unit	Source
chl	-3463.00	kJ/mol	NIST Webbook
gf	-404.52	kJ/mol	Joback Method
hf	-589.37	kJ/mol	Joback Method
hfus	11.30	kJ/mol	Joback Method
hvap	48.25	kJ/mol	Joback Method
log10ws	-0.13		Crippen Method
logp	0.113		Crippen Method
mcvol	113.510	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
tb	519.12	K	Joback Method
tc	726.97	K	Joback Method
tf	354.81	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.03	J/mol×K	519.12	Joback Method
cpg	273.84	J/mol×K	553.76	Joback Method
cpg	283.97	J/mol×K	588.40	Joback Method
cpg	293.50	J/mol×K	623.05	Joback Method
cpg	302.53	J/mol×K	657.69	Joback Method
cpg	311.14	J/mol×K	692.33	Joback Method
cpg	319.40	J/mol×K	726.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6914712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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

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