4-Cyclohexene-1,2-dicarboxylic acid, dimethyl ester

Other names: Dimethyl 4-cyclohexene-1,2-dicarboxylate
RP 1
RP 1 (ester)
4,5-Bis(methoxycarbonyl)cyclohexene

Inchi: InChI=1S/C10H14O4/c1-13-9(11)7-5-3-4-6-8(7)10(12)14-2/h3-4,7-8H,5-6H2,1-2H3

InchiKey: DVVAGRMJGUQHLI-UHFFFAOYSA-N

Formula: C10H14O4

SMILES: COC(=O)C1CC=CCC1C(=O)OC

Mol. weight [g/mol]: 198.22

CAS: 7500-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-387.82	kJ/mol	Joback Method
hf	-647.57	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	56.58	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	0.915		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	594.82	K	Joback Method
tc	807.95	K	Joback Method
tf	350.68	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.01	J/mol×K	594.82	Joback Method
cpg	401.54	J/mol×K	630.34	Joback Method
cpg	416.21	J/mol×K	665.86	Joback Method
cpg	430.02	J/mol×K	701.39	Joback Method
cpg	442.96	J/mol×K	736.91	Joback Method

cpg	455.01	J/mol×K	772.43	Joback Method
cpg	466.18	J/mol×K	807.95	Joback Method
dvisc	0.0018829	Pa×s	350.68	Joback Method
dvisc	0.0011143	Pa×s	391.37	Joback Method
dvisc	0.0007279	Pa×s	432.06	Joback Method
dvisc	0.0005117	Pa×s	472.75	Joback Method
dvisc	0.0003803	Pa×s	513.44	Joback Method
dvisc	0.0002953	Pa×s	554.13	Joback Method
dvisc	0.0002374	Pa×s	594.82	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=C7500552&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

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