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

Inchi: InChI=1S/C11H16O4/c1-7-4-5-8(10(12)14-2)9(6-7)11(13)15-3/h4,8-9H,5-6H2,1-3H3
InchiKey: GODQWBQDOFWJQS-UHFFFAOYSA-N
Formula: C11H16O4
SMILES: COC(=O)C1CC=C(C)CC1C(=O)OC
Mol. weight [g/mol]: 212.24
CAS: 86905-77-3

Physical Properties

Property code	Value	Unit	Source
gf	-389.03	kJ/mol	Joback Method
hf	-679.68	kJ/mol	Joback Method
hfus	23.56	kJ/mol	Joback Method
hvap	59.47	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.305		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1442.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1436.00		NIST Webbook
tb	622.68	K	Joback Method
tc	833.27	K	Joback Method
tf	374.47	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.53	J/mol×K	622.68	Joback Method
cpg	506.38	J/mol×K	798.18	Joback Method
cpg	494.00	J/mol×K	763.08	Joback Method
cpg	480.72	J/mol×K	727.98	Joback Method
cpg	466.54	J/mol×K	692.88	Joback Method

cpg	451.47	J/mol×K	657.78	Joback Method
cpg	517.83	J/mol×K	833.27	Joback Method
dvisc	0.0002146	Pa×s	622.68	Joback Method
dvisc	0.0002640	Pa×s	581.31	Joback Method
dvisc	0.0003352	Pa×s	539.94	Joback Method
dvisc	0.0004429	Pa×s	498.58	Joback Method
dvisc	0.0006153	Pa×s	457.21	Joback Method
dvisc	0.0009128	Pa×s	415.84	Joback Method
dvisc	0.0014773	Pa×s	374.47	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=C86905773&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