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

Inchi: InChI=1S/C10H13ClO4/c1-14-9(12)7-4-3-6(11)5-8(7)10(13)15-2/h3,7-8H,4-5H2,1-2H3
InchiKey: FIYAIUGEFLHXEI-UHFFFAOYSA-N
Formula: C10H13ClO4
SMILES: COC(=O)C1CC=C(Cl)CC1C(=O)OC
Mol. weight [g/mol]: 232.66

Physical Properties

Property code	Value	Unit	Source
gf	-409.38	kJ/mol	Joback Method
hf	-674.78	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	61.62	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.481		Crippen Method
mcvol	163.720	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	637.23	K	Joback Method
tc	854.93	K	Joback Method
tf	393.12	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.88	J/mol×K	637.23	Joback Method
cpg	427.25	J/mol×K	673.51	Joback Method
cpg	440.76	J/mol×K	709.80	Joback Method
cpg	453.38	J/mol×K	746.08	Joback Method
cpg	465.12	J/mol×K	782.37	Joback Method

cpg	475.94	J/mol×K	818.65	Joback Method
cpg	485.85	J/mol×K	854.93	Joback Method
dvisc	0.0014244	Pa×s	393.12	Joback Method
dvisc	0.0009075	Pa×s	433.81	Joback Method
dvisc	0.0006247	Pa×s	474.49	Joback Method
dvisc	0.0004561	Pa×s	515.17	Joback Method
dvisc	0.0003487	Pa×s	555.86	Joback Method
dvisc	0.0002766	Pa×s	596.55	Joback Method
dvisc	0.0002259	Pa×s	637.23	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R33890&Units=SI

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