1,4-Cyclohexanedicarboxylic acid, dimethyl ester

Other names: Dimethyl hexahydroterephthalate
Dimethyl 1,4-cyclohexanedicarboxylate
1,4-Cyclohexanedicarboxylic dimethyl ester
Dimethyl 1,4-cyclohexanedicarboxylate,c&t
1,4-Cyclohexanedicarboxylic acid dimethyl ester,c&t
dimethyl cyclohexane-1,4-dicarboxylate

Inchi: InChI=1S/C10H16O4/c1-13-9(11)7-3-5-8(6-4-7)10(12)14-2/h7-8H,3-6H2,1-2H3

InchiKey: LNGAGQAGYITKCW-UHFFFAOYSA-N

Formula: C10H16O4

SMILES: COC(=O)C1CCC(C(=O)OC)CC1

Mol. weight [g/mol]: 200.23

CAS: 94-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-417.78	kJ/mol	Joback Method
hf	-705.35	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.139		Crippen Method
mcvol	155.780	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	595.66	K	Joback Method
tc	806.87	K	Joback Method
tf	349.92	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.56	J/mol×K	595.66	Joback Method
cpg	423.19	J/mol×K	630.86	Joback Method
cpg	438.92	J/mol×K	666.06	Joback Method

cpg	453.76	J/mol×K	701.26	Joback Method
cpg	467.69	J/mol×K	736.46	Joback Method
cpg	480.69	J/mol×K	771.67	Joback Method
cpg	492.77	J/mol×K	806.87	Joback Method
dvisc	0.0020866	Pa×s	349.92	Joback Method
dvisc	0.0011937	Pa×s	390.88	Joback Method
dvisc	0.0007592	Pa×s	431.83	Joback Method
dvisc	0.0005222	Pa×s	472.79	Joback Method
dvisc	0.0003813	Pa×s	513.75	Joback Method
dvisc	0.0002916	Pa×s	554.70	Joback Method
dvisc	0.0002314	Pa×s	595.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	1.50	NIST Webbook

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=C94600&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume