

cis-Cyclohexane-1,3-dicarboxylic acid dimethyl ester

Inchi:	InChI=1S/C10H16O4/c1-13-9(11)7-4-3-5-8(6-7)10(12)14-2/h7-8H,3-6H2,1-2H3/t7-,8+
InchiKey:	BZUOYGUOKMUSPA-OCAPTIKFSA-N
Formula:	C10H16O4
SMILES:	COC(=O)C1CCCC(C(=O)OC)C1
Mol. weight [g/mol]:	200.23
CAS:	6998-82-9

Physical Properties

Property code	Value	Unit	Source
chl	-5375.44	kJ/mol	NIST Webbook
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	536.20	K	NIST Webbook
tc	806.87	K	Joback Method
tf	349.92	K	Joback Method
vc	0.576	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.56	J/molxK	595.66	Joback Method
cpg	423.19	J/molxK	630.86	Joback Method
cpg	438.92	J/molxK	666.06	Joback Method
cpg	453.76	J/molxK	701.26	Joback Method
cpg	467.69	J/molxK	736.46	Joback Method
cpg	480.69	J/molxK	771.67	Joback Method
cpg	492.77	J/molxK	806.87	Joback Method
dvisc	0.0020866	Paxs	349.92	Joback Method

dvisc	0.0011937	Paxs	390.88	Joback Method
dvisc	0.0007592	Paxs	431.83	Joback Method
dvisc	0.0005222	Paxs	472.79	Joback Method
dvisc	0.0003813	Paxs	513.75	Joback Method
dvisc	0.0002916	Paxs	554.70	Joback Method
dvisc	0.0002314	Paxs	595.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	2.70	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=C6998829&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chl:	Standard liquid enthalpy of combustion
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
mccvol:	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

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