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

Inchi: InChI=1S/C12H20O4/c1-3-15-11(13)9-6-5-7-10(8-9)12(14)16-4-2/h9-10H,3-8H2,1-2H3/t9

InchiKey: MAQGUOIUBYAVNL-AOOOYVTPSA-N

Formula: C12H20O4

SMILES: CCOC(=O)C1CCCC(C(=O)OCC)C1

Mol. weight [g/mol]: 228.28

CAS: 62059-56-7

Physical Properties

Property code	Value	Unit	Source
chl	-6647.00 ± 13.00	kJ/mol	NIST Webbook
gf	-400.94	kJ/mol	Joback Method
hf	-746.63	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.919		Crippen Method
mcvol	183.960	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
tb	641.42	K	Joback Method
tc	846.20	K	Joback Method
tf	372.46	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.57	J/mol×K	641.42	Joback Method
cpg	527.23	J/mol×K	675.55	Joback Method
cpg	543.90	J/mol×K	709.68	Joback Method
cpg	559.58	J/mol×K	743.81	Joback Method
cpg	574.26	J/mol×K	777.94	Joback Method
cpg	587.94	J/mol×K	812.07	Joback Method
cpg	600.62	J/mol×K	846.20	Joback Method
dvisc	0.0019188	Pa×s	372.46	Joback Method

dvisc	0.0010612	Pa×s	417.29	Joback Method
dvisc	0.0006584	Pa×s	462.11	Joback Method
dvisc	0.0004445	Pa×s	506.94	Joback Method
dvisc	0.0003198	Pa×s	551.77	Joback Method
dvisc	0.0002418	Pa×s	596.59	Joback Method
dvisc	0.0001901	Pa×s	641.42	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=C62059567&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume