1,2-Cyclohexanedicarboxylic acid, ethyl isopropyl ester

Inchi: InChI=1S/C13H22O4/c1-4-16-12(14)10-7-5-6-8-11(10)13(15)17-9(2)3/h9-11H,4-8H2,1-3

InchiKey: SRBJOBVOYKMWDX-UHFFFAOYSA-N

Formula: C13H22O4

SMILES: CCOC(=O)C1CCCCC1C(=O)OC(C)C

Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-394.96	kJ/mol	Joback Method
hf	-772.55	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	62.58	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.308		Crippen Method
mcvol	198.050	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	663.86	K	Joback Method
tc	869.51	K	Joback Method
tf	368.73	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.65	J/mol×K	663.86	Joback Method
cpg	582.05	J/mol×K	698.13	Joback Method
cpg	599.36	J/mol×K	732.41	Joback Method
cpg	615.59	J/mol×K	766.68	Joback Method
cpg	630.75	J/mol×K	800.96	Joback Method
cpg	644.82	J/mol×K	835.23	Joback Method
cpg	657.80	J/mol×K	869.51	Joback Method
dvisc	0.0022079	Pa×s	368.73	Joback Method

dvisc	0.0010990	Pa×s	417.92	Joback Method
dvisc	0.0006337	Pa×s	467.11	Joback Method
dvisc	0.0004058	Pa×s	516.30	Joback Method
dvisc	0.0002808	Pa×s	565.48	Joback Method
dvisc	0.0002061	Pa×s	614.67	Joback Method
dvisc	0.0001584	Pa×s	663.86	Joback Method

Sources

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=U339635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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