1,2-Cyclohexanedicarboxylic acid, isohexyl isopropyl ester

Inchi: InChI=1S/C17H30O4/c1-12(2)8-7-11-20-16(18)14-9-5-6-10-15(14)17(19)21-13(3)4/h12-1

InchiKey: ONUIWTQGPQZMLW-UHFFFAOYSA-N

Formula: C17H30O4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)OC(C)C

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-363.72	kJ/mol	Joback Method
hf	-860.39	kJ/mol	Joback Method
hfus	31.22	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.724		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
tb	754.94	K	Joback Method
tc	955.18	K	Joback Method
tf	398.81	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.61	J/mol×K	754.94	Joback Method
cpg	810.05	J/mol×K	788.31	Joback Method
cpg	828.22	J/mol×K	821.69	Joback Method
cpg	845.14	J/mol×K	855.06	Joback Method
cpg	860.80	J/mol×K	888.43	Joback Method
cpg	875.23	J/mol×K	921.80	Joback Method
cpg	888.42	J/mol×K	955.18	Joback Method
dvisc	0.0019397	Pa×s	398.81	Joback Method

dvisc	0.0008336	Pa×s	458.17	Joback Method
dvisc	0.0004348	Pa×s	517.52	Joback Method
dvisc	0.0002593	Pa×s	576.88	Joback Method
dvisc	0.0001703	Pa×s	636.23	Joback Method
dvisc	0.0001202	Pa×s	695.59	Joback Method
dvisc	0.0000896	Pa×s	754.94	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=U339639&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume