

1,2-Cyclohexanedicarboxylic acid, diisopropyl ester

Inchi:	InChI=1S/C14H24O4/c1-9(2)17-13(15)11-7-5-6-8-12(11)14(16)18-10(3)4/h9-12H,5-8H2,
InchiKey:	HFVJRYILMUSLFV-UHFFFAOYSA-N
Formula:	C14H24O4
SMILES:	CC(C)OC(=O)C1CCCCC1C(=O)OC(C)C
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-388.98	kJ/mol	Joback Method
hf	-798.47	kJ/mol	Joback Method
hfus	23.45	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.696		Crippen Method
mvol	212.140	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
tb	686.30	K	Joback Method
tc	892.79	K	Joback Method
tf	365.00	K	Joback Method
vc	0.787	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.04	J/molxK	686.30	Joback Method
cpg	638.07	J/molxK	720.72	Joback Method
cpg	655.92	J/molxK	755.13	Joback Method
cpg	672.62	J/molxK	789.55	Joback Method
cpg	688.14	J/molxK	823.96	Joback Method
cpg	702.51	J/molxK	858.38	Joback Method
cpg	715.72	J/molxK	892.79	Joback Method
dvisc	0.0025535	Paxs	365.00	Joback Method

dvisc	0.0011333	Paxs	418.55	Joback Method
dvisc	0.0006048	Paxs	472.10	Joback Method
dvisc	0.0003668	Paxs	525.65	Joback Method
dvisc	0.0002440	Paxs	579.20	Joback Method
dvisc	0.0001739	Paxs	632.75	Joback Method
dvisc	0.0001307	Paxs	686.30	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=U339648&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

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