1,2-Cyclohexanedicarboxylic acid, isobutyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C19H32O4/c1-13(2)12-22-18(20)15-9-5-6-10-16(15)19(21)23-17-11-7-4-8-14(1

InchiKey: RYJARZHRNSBYFI-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-327.70	kJ/mol	Joback Method
hf	-862.41	kJ/mol	Joback Method
hfus	32.83	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.114		Crippen Method
mcvol	271.730	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	816.02	K	Joback Method
tc	1034.14	K	Joback Method
tf	439.49	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.38	J/mol×K	816.02	Joback Method
cpg	930.62	J/mol×K	852.37	Joback Method
cpg	950.07	J/mol×K	888.73	Joback Method
cpg	967.74	J/mol×K	925.08	Joback Method
cpg	983.64	J/mol×K	961.43	Joback Method
cpg	997.79	J/mol×K	997.78	Joback Method
cpg	1010.21	J/mol×K	1034.14	Joback Method
dvisc	0.0015595	Pa×s	439.49	Joback Method

dvisc	0.0007390	Pa×s	502.25	Joback Method
dvisc	0.0004133	Pa×s	565.00	Joback Method
dvisc	0.0002597	Pa×s	627.75	Joback Method
dvisc	0.0001775	Pa×s	690.51	Joback Method
dvisc	0.0001293	Pa×s	753.26	Joback Method
dvisc	0.0000989	Pa×s	816.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U339876&Units=SI

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