1,2-Cyclohexanedicarboxylic acid, 4-chloro-3-methylphenyl isobutyl ester

Inchi: InChI=1S/C19H25ClO4/c1-12(2)11-23-18(21)15-6-4-5-7-16(15)19(22)24-14-8-9-17(20)13

InchiKey: DFPHCPYOPJAKAA-UHFFFAOYSA-N

Formula: C19H25ClO4

SMILES: Cc1cc(OC(=O)C2CCCCC2C(=O)OCC(C)C)ccc1Cl

Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-263.22	kJ/mol	Joback Method
hf	-698.54	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	83.92	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.559		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		NIST Webbook
tb	875.21	K	Joback Method
tc	1103.07	K	Joback Method
tf	517.73	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.37	J/mol×K	875.21	Joback Method
cpg	860.23	J/mol×K	913.19	Joback Method
cpg	874.50	J/mol×K	951.16	Joback Method
cpg	887.19	J/mol×K	989.14	Joback Method
cpg	898.32	J/mol×K	1027.12	Joback Method
cpg	907.92	J/mol×K	1065.10	Joback Method
cpg	915.99	J/mol×K	1103.07	Joback Method
dvisc	0.0006484	Pa×s	517.73	Joback Method

dvisc	0.0003672	Pa×s	577.31	Joback Method
dvisc	0.0002313	Pa×s	636.89	Joback Method
dvisc	0.0001577	Pa×s	696.47	Joback Method
dvisc	0.0001142	Pa×s	756.05	Joback Method
dvisc	0.0000867	Pa×s	815.63	Joback Method
dvisc	0.0000683	Pa×s	875.21	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=U339685&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