1,2-Cyclohexanedicarboxylic acid, (2-chlorocyclohexyl)methyl isobutyl ester

Inchi: InChI=1S/C19H31ClO4/c1-13(2)11-23-18(21)15-8-4-5-9-16(15)19(22)24-12-14-7-3-6-10-

InchiKey: VITSSUIDGHFLAL-UHFFFAOYSA-N

Formula: C19H31ClO4

SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 358.90

Physical Properties

Property code	Value	Unit	Source
gf	-339.63	kJ/mol	Joback Method
hf	-878.15	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.333		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2463.00		NIST Webbook
tb	853.45	K	Joback Method
tc	1074.95	K	Joback Method
tf	469.41	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.64	J/mol×K	853.45	Joback Method
cpg	1019.46	J/mol×K	1038.03	Joback Method
cpg	1007.27	J/mol×K	1001.12	Joback Method
cpg	993.31	J/mol×K	964.20	Joback Method
cpg	977.56	J/mol×K	927.28	Joback Method
cpg	960.01	J/mol×K	890.37	Joback Method
cpg	1029.89	J/mol×K	1074.95	Joback Method
dvisc	0.0000865	Pa×s	853.45	Joback Method
dvisc	0.0001129	Pa×s	789.44	Joback Method

dvisc	0.0001543	Pa×s	725.44	Joback Method
dvisc	0.0002241	Pa×s	661.43	Joback Method
dvisc	0.0003527	Pa×s	597.42	Joback Method
dvisc	0.0006187	Pa×s	533.42	Joback Method
dvisc	0.0012652	Pa×s	469.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339859&Units=SI
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

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