1,2-Cyclohexanedicarboxylic acid, 2-chlorophenyl isohexyl ester

Inchi: InChI=1S/C20H27ClO4/c1-14(2)8-7-13-24-19(22)15-9-3-4-10-16(15)20(23)25-18-12-6-5-

InchiKey: SIQKPUBVZJPFQD-UHFFFAOYSA-N

Formula: C20H27ClO4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 366.88

Physical Properties

Property code	Value	Unit	Source
gf	-245.17	kJ/mol	Joback Method
hf	-707.71	kJ/mol	Joback Method
hfus	40.36	kJ/mol	Joback Method
hvap	85.48	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.031		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2547.00		NIST Webbook
rinpol	2547.00		NIST Webbook
tb	893.11	K	Joback Method
tc	1118.48	K	Joback Method
tf	516.48	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.16	J/mol×K	893.11	Joback Method
cpg	920.04	J/mol×K	930.67	Joback Method
cpg	934.32	J/mol×K	968.23	Joback Method
cpg	947.02	J/mol×K	1005.80	Joback Method
cpg	958.18	J/mol×K	1043.36	Joback Method
cpg	967.82	J/mol×K	1080.92	Joback Method
cpg	975.98	J/mol×K	1118.48	Joback Method
dvisc	0.0006755	Pa×s	516.48	Joback Method

dvisc	0.0003601	Pa×s	579.25	Joback Method
dvisc	0.0002171	Pa×s	642.02	Joback Method
dvisc	0.0001432	Pa×s	704.79	Joback Method
dvisc	0.0001011	Pa×s	767.57	Joback Method
dvisc	0.0000753	Pa×s	830.34	Joback Method
dvisc	0.0000584	Pa×s	893.11	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=U339586&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