1,2-Cyclohexanedicarboxylic acid, 4-chloro-2-methylphenyl isohexyl ester

Inchi: InChI=1S/C21H29ClO4/c1-14(2)7-6-12-25-20(23)17-8-4-5-9-18(17)21(24)26-19-11-10-16

InchiKey: HISCKIQTJMXHFR-UHFFFAOYSA-N

Formula: C21H29ClO4

SMILES: Cc1cc(Cl)ccc1OC(=O)C1CCCCC1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 380.91

Physical Properties

Property code	Value	Unit	Source
gf	-246.38	kJ/mol	Joback Method
hf	-739.82	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	88.37	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.340		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2657.00		NIST Webbook
rinpol	2657.00		NIST Webbook
tb	920.97	K	Joback Method
tc	1146.11	K	Joback Method
tf	540.27	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.76	J/mol×K	920.97	Joback Method
cpg	1024.56	J/mol×K	1108.59	Joback Method
cpg	1015.40	J/mol×K	1071.07	Joback Method
cpg	1004.66	J/mol×K	1033.54	Joback Method
cpg	992.33	J/mol×K	996.02	Joback Method
cpg	978.37	J/mol×K	958.49	Joback Method
cpg	1032.17	J/mol×K	1146.11	Joback Method
dvisc	0.0000517	Pa×s	920.97	Joback Method

dvisc	0.0000660	Pa×s	857.52	Joback Method
dvisc	0.0000876	Pa×s	794.07	Joback Method
dvisc	0.0001222	Pa×s	730.62	Joback Method
dvisc	0.0001815	Pa×s	667.17	Joback Method
dvisc	0.0002930	Pa×s	603.72	Joback Method
dvisc	0.0005294	Pa×s	540.27	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=U339792&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