1,2-Cyclohexanedicarboxylic acid, di(4-chloro-3-methylphenyl) ester

Inchi: InChI=1S/C22H22Cl2O4/c1-13-11-15(7-9-19(13)23)27-21(25)17-5-3-4-6-18(17)22(26)28
InchiKey: FBPJTZJTIUOXOI-UHFFFAOYSA-N
Formula: C22H22Cl2O4
SMILES: Cc1cc(OC(=O)C2CCCCC2C(=O)Oc2ccc(Cl)c(C)c2)ccc1Cl
Mol. weight [g/mol]: 421.31

Physical Properties

Property code	Value	Unit	Source
gf	-154.30	kJ/mol	Joback Method
hf	-557.33	kJ/mol	Joback Method
hfus	46.14	kJ/mol	Joback Method
hvap	98.97	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	5.928		Crippen Method
mcvol	301.820	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1018.36	K	Joback Method
tc	1270.80	K	Joback Method
tf	647.92	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.71	J/mol×K	1018.36	Joback Method
cpg	968.43	J/mol×K	1228.72	Joback Method
cpg	965.17	J/mol×K	1186.65	Joback Method
cpg	960.11	J/mol×K	1144.58	Joback Method
cpg	953.20	J/mol×K	1102.51	Joback Method
cpg	944.41	J/mol×K	1060.43	Joback Method
cpg	969.90	J/mol×K	1270.80	Joback Method
dvisc	0.0000461	Pa×s	1018.36	Joback Method

dvisc	0.0000565	Pa×s	956.62	Joback Method
dvisc	0.0000711	Pa×s	894.88	Joback Method
dvisc	0.0000927	Pa×s	833.14	Joback Method
dvisc	0.0001260	Pa×s	771.40	Joback Method
dvisc	0.0001808	Pa×s	709.66	Joback Method
dvisc	0.0002778	Pa×s	647.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339689&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