cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(4-chloro-3-methylphenyl) ester

Inchi: InChI=1S/C22H20Cl2O4/c1-13-11-15(7-9-19(13)23)27-21(25)17-5-3-4-6-18(17)22(26)28
InchiKey: RQGDIHNJOSPEBX-UHFFFAOYSA-N
Formula: C22H20Cl2O4
SMILES: Cc1cc(OC(=O)C2CC=CCC2C(=O)Oc2ccc(Cl)c(C)c2)ccc1Cl
Mol. weight [g/mol]: 419.30

Physical Properties

Property code	Value	Unit	Source
gf	-124.34	kJ/mol	Joback Method
hf	-499.55	kJ/mol	Joback Method
hfus	47.36	kJ/mol	Joback Method
hvap	99.26	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.704		Crippen Method
mcvol	297.520	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	3174.00		NIST Webbook
rinpol	3174.00		NIST Webbook
tb	1017.52	K	Joback Method
tc	1271.19	K	Joback Method
tf	648.68	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.87	J/mol×K	1017.52	Joback Method
cpg	911.98	J/mol×K	1059.80	Joback Method
cpg	920.25	J/mol×K	1102.08	Joback Method
cpg	926.72	J/mol×K	1144.35	Joback Method
cpg	931.43	J/mol×K	1186.63	Joback Method
cpg	934.40	J/mol×K	1228.91	Joback Method
cpg	935.68	J/mol×K	1271.19	Joback Method
dvisc	0.0002874	Pa×s	648.68	Joback Method

dvisc	0.0001899	Pa×s	710.15	Joback Method
dvisc	0.0001341	Pa×s	771.63	Joback Method
dvisc	0.0000997	Pa×s	833.10	Joback Method
dvisc	0.0000771	Pa×s	894.57	Joback Method
dvisc	0.0000617	Pa×s	956.05	Joback Method
dvisc	0.0000507	Pa×s	1017.52	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U382659&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