

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

Inchi: InChI=1S/C22H22Cl2O4/c1-13-11-15(23)7-9-19(13)27-21(25)17-5-3-4-6-18(17)22(26)28

InchiKey: BFWCPJYLRXSIHE-UHFFFAOYSA-N

Formula: C22H22Cl2O4

SMILES: Cc1cc(Cl)ccc1OC(=O)C1CCCCC1C(=O)Oc1ccc(Cl)cc1C

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
mvol	301.820	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	3171.00		NIST Webbook
rinpol	3171.00		NIST Webbook
tb	1018.36	K	Joback Method
tc	1270.80	K	Joback Method
tf	647.92	K	Joback Method
vc	1.129	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.71	J/molxK	1018.36	Joback Method
cpg	944.41	J/molxK	1060.43	Joback Method
cpg	953.20	J/molxK	1102.51	Joback Method
cpg	960.11	J/molxK	1144.58	Joback Method
cpg	965.17	J/molxK	1186.65	Joback Method
cpg	968.43	J/molxK	1228.72	Joback Method
cpg	969.90	J/molxK	1270.80	Joback Method
dvisc	0.0002778	Paxs	647.92	Joback Method

dvisc	0.0001808	Paxs	709.66	Joback Method
dvisc	0.0001260	Paxs	771.40	Joback Method
dvisc	0.0000927	Paxs	833.14	Joback Method
dvisc	0.0000711	Paxs	894.88	Joback Method
dvisc	0.0000565	Paxs	956.62	Joback Method
dvisc	0.0000461	Paxs	1018.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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