

1,2-Cyclohexanedicarboxylic acid, di(3-chlorophenyl) ester

Inchi:	InChI=1S/C20H18Cl2O4/c21-13-5-3-7-15(11-13)25-19(23)17-9-1-2-10-18(17)20(24)26-1
InchiKey:	OQCLQCAWNUZKBD-UHFFFAOYSA-N
Formula:	C20H18Cl2O4
SMILES:	O=C(Oc1cccc(Cl)c1)C1CCCCC1C(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	393.26

Physical Properties

Property code	Value	Unit	Source
gf	-151.88	kJ/mol	Joback Method
hf	-493.11	kJ/mol	Joback Method
hfus	41.73	kJ/mol	Joback Method
hvap	93.19	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.311		Crippen Method
mcvol	273.640	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	3016.00		NIST Webbook
rinpol	3016.00		NIST Webbook
tb	962.64	K	Joback Method
tc	1219.03	K	Joback Method
tf	600.34	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.14	J/molxK	962.64	Joback Method
cpg	832.68	J/molxK	1005.37	Joback Method
cpg	842.40	J/molxK	1048.10	Joback Method
cpg	850.34	J/molxK	1090.83	Joback Method
cpg	856.56	J/molxK	1133.56	Joback Method
cpg	861.09	J/molxK	1176.29	Joback Method
cpg	863.99	J/molxK	1219.03	Joback Method
dvisc	0.0004102	Paxs	600.34	Joback Method

dvisc	0.0002553	Paxs	660.72	Joback Method
dvisc	0.0001721	Paxs	721.11	Joback Method
dvisc	0.0001233	Paxs	781.49	Joback Method
dvisc	0.0000926	Paxs	841.87	Joback Method
dvisc	0.0000723	Paxs	902.26	Joback Method
dvisc	0.0000582	Paxs	962.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339696&Units=SI

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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