1,2-Cyclohexanedicarboxylic acid, propyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C17H19Cl3O4/c1-2-7-23-16(21)11-5-3-4-6-12(11)17(22)24-15-13(19)8-10(18)9

InchiKey: GLZUTZREYQLZHV-UHFFFAOYSA-N

Formula: C17H19Cl3O4

SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 393.69

Physical Properties

Property code	Value	Unit	Source
gf	-311.11	kJ/mol	Joback Method
hf	-694.93	kJ/mol	Joback Method
hfus	43.73	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.312		Crippen Method
mcvol	267.370	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	909.73	K	Joback Method
tc	1145.97	K	Joback Method
tf	582.55	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.10	J/mol×K	909.73	Joback Method
cpg	820.98	J/mol×K	1106.59	Joback Method
cpg	814.63	J/mol×K	1067.22	Joback Method
cpg	806.78	J/mol×K	1027.85	Joback Method
cpg	797.41	J/mol×K	988.48	Joback Method
cpg	786.52	J/mol×K	949.10	Joback Method
cpg	825.83	J/mol×K	1145.97	Joback Method
dvisc	0.0000752	Pa×s	909.73	Joback Method

dvisc	0.0000922	Pa×s	855.20	Joback Method
dvisc	0.0001163	Pa×s	800.67	Joback Method
dvisc	0.0001518	Pa×s	746.14	Joback Method
dvisc	0.0002067	Pa×s	691.61	Joback Method
dvisc	0.0002965	Pa×s	637.08	Joback Method
dvisc	0.0004553	Pa×s	582.55	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=U339806&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