1,2-Cyclohexanedicarboxylic acid, 4-chlorophenyl pentyl ester

Inchi: InChI=1S/C19H25ClO4/c1-2-3-6-13-23-18(21)16-7-4-5-8-17(16)19(22)24-15-11-9-14(20)
InchiKey: IOFQNQLRZAOBIB-UHFFFAOYSA-N
Formula: C19H25ClO4
SMILES: CCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-251.15	kJ/mol	Joback Method
hf	-681.79	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.785		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	870.67	K	Joback Method
tc	1094.87	K	Joback Method
tf	520.21	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.76	J/mol×K	870.67	Joback Method
cpg	860.57	J/mol×K	908.04	Joback Method
cpg	874.86	J/mol×K	945.40	Joback Method
cpg	887.64	J/mol×K	982.77	Joback Method
cpg	898.94	J/mol×K	1020.14	Joback Method
cpg	908.79	J/mol×K	1057.50	Joback Method
cpg	917.20	J/mol×K	1094.87	Joback Method
dvisc	0.0006746	Pa×s	520.21	Joback Method

dvisc	0.0003868	Pa×s	578.62	Joback Method
dvisc	0.0002456	Pa×s	637.03	Joback Method
dvisc	0.0001683	Pa×s	695.44	Joback Method
dvisc	0.0001223	Pa×s	753.85	Joback Method
dvisc	0.0000930	Pa×s	812.26	Joback Method
dvisc	0.0000734	Pa×s	870.67	Joback Method

Sources

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=U339682&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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