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

Inchi: InChI=1S/C17H21ClO4/c1-2-11-21-16(19)14-5-3-4-6-15(14)17(20)22-13-9-7-12(18)8-10-

InchiKey: QNBQXLUZHWOQSH-UHFFFAOYSA-N

Formula: C17H21ClO4

SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-267.99	kJ/mol	Joback Method
hf	-640.51	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.005		Crippen Method
mcvol	242.890	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	824.91	K	Joback Method
tc	1053.94	K	Joback Method
tf	497.67	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.03	J/mol×K	824.91	Joback Method
cpg	793.83	J/mol×K	1015.77	Joback Method
cpg	783.78	J/mol×K	977.60	Joback Method
cpg	772.29	J/mol×K	939.42	Joback Method
cpg	759.35	J/mol×K	901.25	Joback Method
cpg	744.93	J/mol×K	863.08	Joback Method
cpg	802.47	J/mol×K	1053.94	Joback Method
dvisc	0.0000961	Pa×s	824.91	Joback Method

dvisc	0.0001210	Pa×s	770.37	Joback Method
dvisc	0.0001577	Pa×s	715.83	Joback Method
dvisc	0.0002147	Pa×s	661.29	Joback Method
dvisc	0.0003089	Pa×s	606.75	Joback Method
dvisc	0.0004777	Pa×s	552.21	Joback Method
dvisc	0.0008127	Pa×s	497.67	Joback Method

Sources

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=U339679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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