1,2-Cyclohexanedicarboxylic acid, 2-chlorophenyl pentadecyl ester

Inchi: InChI=1S/C29H45ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-23-33-28(31)24-19-14-15-20-

InchiKey: GIALXPAJIWDMQC-UHFFFAOYSA-N

Formula: C29H45ClO4

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 493.12

Physical Properties

Property code	Value	Unit	Source
gf	-166.95	kJ/mol	Joback Method
hf	-888.19	kJ/mol	Joback Method
hfus	67.19	kJ/mol	Joback Method
hvap	105.90	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.686		Crippen Method
mcvol	411.970	ml/mol	McGowan Method
pc	835.79	kPa	Joback Method
rinpol	3567.00		NIST Webbook
tb	1099.47	K	Joback Method
tc	1348.99	K	Joback Method
tf	632.91	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1454.10	J/mol×K	1099.47	Joback Method
cpg	1469.08	J/mol×K	1141.06	Joback Method
cpg	1481.88	J/mol×K	1182.64	Joback Method
cpg	1492.59	J/mol×K	1224.23	Joback Method
cpg	1501.29	J/mol×K	1265.81	Joback Method
cpg	1508.07	J/mol×K	1307.40	Joback Method
cpg	1513.01	J/mol×K	1348.99	Joback Method
dvisc	0.0002139	Pa×s	632.91	Joback Method
dvisc	0.0001107	Pa×s	710.67	Joback Method

dvisc	0.0000653	Pa×s	788.43	Joback Method
dvisc	0.0000423	Pa×s	866.19	Joback Method
dvisc	0.0000295	Pa×s	943.95	Joback Method
dvisc	0.0000217	Pa×s	1021.71	Joback Method
dvisc	0.0000167	Pa×s	1099.47	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=U339591&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