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

Inchi: InChI=1S/C25H37ClO4/c1-2-3-4-5-6-7-8-9-14-19-29-24(27)20-15-10-11-16-21(20)25(28)

InchiKey: IXBJYWHFUVBKIA-UHFFFAOYSA-N

Formula: C25H37ClO4

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

Mol. weight [g/mol]: 437.01

Physical Properties

Property code	Value	Unit	Source
gf	-200.63	kJ/mol	Joback Method
hf	-805.63	kJ/mol	Joback Method
hfus	56.83	kJ/mol	Joback Method
hvap	97.00	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.126		Crippen Method
mcvol	355.610	ml/mol	McGowan Method
pc	1057.57	kPa	Joback Method
rinpol	3131.00		NIST Webbook
rinpol	3131.00		NIST Webbook
tb	1007.95	K	Joback Method
tc	1235.71	K	Joback Method
tf	587.83	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.00	J/mol×K	1007.95	Joback Method
cpg	1221.24	J/mol×K	1045.91	Joback Method
cpg	1234.69	J/mol×K	1083.87	Joback Method
cpg	1246.42	J/mol×K	1121.83	Joback Method
cpg	1256.46	J/mol×K	1159.79	Joback Method
cpg	1264.88	J/mol×K	1197.75	Joback Method
cpg	1271.71	J/mol×K	1235.71	Joback Method
dvisc	0.0003512	Pa×s	587.83	Joback Method

dvisc	0.0001887	Pa×s	657.85	Joback Method
dvisc	0.0001142	Pa×s	727.87	Joback Method
dvisc	0.0000755	Pa×s	797.89	Joback Method
dvisc	0.0000534	Pa×s	867.91	Joback Method
dvisc	0.0000397	Pa×s	937.93	Joback Method
dvisc	0.0000308	Pa×s	1007.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339589&Units=SI
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

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