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

Inchi: InChI=1S/C26H39ClO4/c1-2-3-4-5-6-7-8-9-10-15-20-30-25(28)21-16-11-12-17-22(21)26(

InchiKey: SANGHKSWEYCKSW-UHFFFAOYSA-N

Formula: C26H39ClO4

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

Mol. weight [g/mol]: 451.04

Physical Properties

Property code	Value	Unit	Source
gf	-192.21	kJ/mol	Joback Method
hf	-826.27	kJ/mol	Joback Method
hfus	59.42	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.516		Crippen Method
mcvol	369.700	ml/mol	McGowan Method
pc	994.51	kPa	Joback Method
rinpol	3233.00		NIST Webbook
rinpol	3233.00		NIST Webbook
tb	1030.83	K	Joback Method
tc	1262.35	K	Joback Method
tf	599.10	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1267.65	J/mol×K	1030.83	Joback Method
cpg	1325.41	J/mol×K	1223.77	Joback Method
cpg	1317.35	J/mol×K	1185.18	Joback Method
cpg	1307.60	J/mol×K	1146.59	Joback Method
cpg	1296.10	J/mol×K	1108.00	Joback Method
cpg	1282.80	J/mol×K	1069.42	Joback Method
cpg	1331.84	J/mol×K	1262.35	Joback Method
dvisc	0.0000265	Pa×s	1030.83	Joback Method

dvisc	0.0000342	Pa×s	958.87	Joback Method
dvisc	0.0000461	Pa×s	886.92	Joback Method
dvisc	0.0000655	Pa×s	814.96	Joback Method
dvisc	0.0000996	Pa×s	743.01	Joback Method
dvisc	0.0001657	Pa×s	671.05	Joback Method
dvisc	0.0003115	Pa×s	599.10	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=U339590&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