cis-Cyclohex-4-en-1,2-dicarboxylic acid, 4-chloro-3-methylphenyl dodecyl ester

Inchi: InChI=1S/C27H39ClO4/c1-3-4-5-6-7-8-9-10-11-14-19-31-26(29)23-15-12-13-16-24(23)27

InchiKey: PZGNDLBOCJAXHL-UHFFFAOYSA-N

Formula: C27H39ClO4

SMILES: CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 463.05

Physical Properties

Property code	Value	Unit	Source
gf	-163.46	kJ/mol	Joback Method
hf	-800.60	kJ/mol	Joback Method
hfus	62.85	kJ/mol	Joback Method
hvap	102.40	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	7.600		Crippen Method
mcvol	379.490	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
rinpol	3336.00		NIST Webbook
tb	1057.85	K	Joback Method
tc	1295.11	K	Joback Method
tf	623.65	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1295.92	J/mol×K	1057.85	Joback Method
cpg	1310.23	J/mol×K	1097.39	Joback Method
cpg	1322.62	J/mol×K	1136.94	Joback Method
cpg	1333.15	J/mol×K	1176.48	Joback Method
cpg	1341.87	J/mol×K	1216.02	Joback Method
cpg	1348.85	J/mol×K	1255.57	Joback Method
cpg	1354.13	J/mol×K	1295.11	Joback Method
dvisc	0.0002542	Pa×s	623.65	Joback Method
dvisc	0.0001425	Pa×s	696.02	Joback Method

dvisc	0.0000891	Pa×s	768.38	Joback Method
dvisc	0.0000604	Pa×s	840.75	Joback Method
dvisc	0.0000435	Pa×s	913.12	Joback Method
dvisc	0.0000329	Pa×s	985.48	Joback Method
dvisc	0.0000259	Pa×s	1057.85	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=U382656&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