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

Inchi: InChI=1S/C29H44O4/c1-2-3-4-5-6-7-8-9-10-16-23-32-28(30)26-21-14-15-22-27(26)29(31

InchiKey: OYQHZDQQFVVJHB-UHFFFAOYSA-N

Formula: C29H44O4

SMILES: CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 456.66

Physical Properties

Property code	Value	Unit	Source
gf	-115.43	kJ/mol	Joback Method
hf	-803.20	kJ/mol	Joback Method
hfus	64.61	kJ/mol	Joback Method
hvap	101.15	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.209		Crippen Method
mcvol	395.430	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	3328.00		NIST Webbook
rinpol	3328.00		NIST Webbook
tb	1056.22	K	Joback Method
tc	1293.87	K	Joback Method
tf	591.23	K	Joback Method
vc	1.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.07	J/mol×K	1056.22	Joback Method
cpg	1415.38	J/mol×K	1095.83	Joback Method
cpg	1429.72	J/mol×K	1135.44	Joback Method
cpg	1442.19	J/mol×K	1175.04	Joback Method
cpg	1452.86	J/mol×K	1214.65	Joback Method
cpg	1461.82	J/mol×K	1254.26	Joback Method
cpg	1469.14	J/mol×K	1293.87	Joback Method
dvisc	0.0003110	Pa×s	591.23	Joback Method

dvisc	0.0001538	Pa×s	668.73	Joback Method
dvisc	0.0000880	Pa×s	746.23	Joback Method
dvisc	0.0000560	Pa×s	823.73	Joback Method
dvisc	0.0000385	Pa×s	901.22	Joback Method
dvisc	0.0000281	Pa×s	978.72	Joback Method
dvisc	0.0000214	Pa×s	1056.22	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=U382783&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