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

Inchi: InChI=1S/C30H46O4/c1-2-3-4-5-6-7-8-9-10-11-17-24-33-29(31)27-22-15-16-23-28(27)30

InchiKey: JVIGWTWTMOCOCP-UHFFFAOYSA-N

Formula: C30H46O4

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

Mol. weight [g/mol]: 470.68

Physical Properties

Property code	Value	Unit	Source
gf	-107.01	kJ/mol	Joback Method
hf	-823.84	kJ/mol	Joback Method
hfus	67.20	kJ/mol	Joback Method
hvap	103.37	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.599		Crippen Method
mcvol	409.520	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3426.00		NIST Webbook
rinpol	3426.00		NIST Webbook
tb	1079.10	K	Joback Method
tc	1323.82	K	Joback Method
tf	602.50	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1461.95	J/mol×K	1079.10	Joback Method
cpg	1478.29	J/mol×K	1119.89	Joback Method
cpg	1492.55	J/mol×K	1160.67	Joback Method
cpg	1504.84	J/mol×K	1201.46	Joback Method
cpg	1515.24	J/mol×K	1242.25	Joback Method
cpg	1523.85	J/mol×K	1283.03	Joback Method
cpg	1530.77	J/mol×K	1323.82	Joback Method
dvisc	0.0002741	Pa×s	602.50	Joback Method

dvisc	0.0001344	Pa×s	681.93	Joback Method
dvisc	0.0000765	Pa×s	761.37	Joback Method
dvisc	0.0000484	Pa×s	840.80	Joback Method
dvisc	0.0000332	Pa×s	920.23	Joback Method
dvisc	0.0000241	Pa×s	999.67	Joback Method
dvisc	0.0000184	Pa×s	1079.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382784&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