cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexyl undecyl ester

Inchi: InChI=1S/C25H44O4/c1-3-5-7-9-10-11-12-13-17-21-29-25(27)23-19-15-14-18-22(23)24(

InchiKey: VACVHLOQJNPQOU-UHFFFAOYSA-N

Formula: C25H44O4

SMILES: CCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCC

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-261.52	kJ/mol	Joback Method
hf	-957.17	kJ/mol	Joback Method
hfus	60.21	kJ/mol	Joback Method
hvap	89.97	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.766		Crippen Method
mcvol	362.830	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpol	2781.00		NIST Webbook
tb	938.02	K	Joback Method
tc	1148.40	K	Joback Method
tf	519.73	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.69	J/mol×K	938.02	Joback Method
cpg	1270.92	J/mol×K	973.08	Joback Method
cpg	1288.52	J/mol×K	1008.15	Joback Method
cpg	1304.50	J/mol×K	1043.21	Joback Method
cpg	1318.92	J/mol×K	1078.27	Joback Method
cpg	1331.81	J/mol×K	1113.34	Joback Method
cpg	1343.20	J/mol×K	1148.40	Joback Method
dvisc	0.0005756	Pa×s	519.73	Joback Method
dvisc	0.0002790	Pa×s	589.45	Joback Method

dvisc	0.0001577	Pa×s	659.16	Joback Method
dvisc	0.0000994	Pa×s	728.88	Joback Method
dvisc	0.0000679	Pa×s	798.59	Joback Method
dvisc	0.0000493	Pa×s	868.31	Joback Method
dvisc	0.0000375	Pa×s	938.02	Joback Method

Sources

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=U382668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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