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

Inchi: InChI=1S/C27H48O4/c1-4-7-8-9-10-11-12-13-14-15-18-21-30-26(28)24-19-16-17-20-25(

InchiKey: QRTDSXVEGOOLIG-UHFFFAOYSA-N

Formula: C27H48O4

SMILES: CCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-247.12	kJ/mol	Joback Method
hf	-1003.73	kJ/mol	Joback Method
hfus	61.86	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.402		Crippen Method
mcvol	391.010	ml/mol	McGowan Method
pc	815.39	kPa	Joback Method
rinpol	2932.00		NIST Webbook
rinpol	2932.00		NIST Webbook
tb	983.34	K	Joback Method
tc	1205.22	K	Joback Method
tf	527.27	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.25	J/mol×K	983.34	Joback Method
cpg	1398.80	J/mol×K	1020.32	Joback Method
cpg	1416.47	J/mol×K	1057.30	Joback Method
cpg	1432.30	J/mol×K	1094.28	Joback Method
cpg	1446.35	J/mol×K	1131.26	Joback Method
cpg	1458.67	J/mol×K	1168.24	Joback Method
cpg	1469.30	J/mol×K	1205.22	Joback Method
dvisc	0.0005083	Pa×s	527.27	Joback Method

dvisc	0.0002251	Pa×s	603.28	Joback Method
dvisc	0.0001197	Pa×s	679.29	Joback Method
dvisc	0.0000722	Pa×s	755.31	Joback Method
dvisc	0.0000478	Pa×s	831.32	Joback Method
dvisc	0.0000339	Pa×s	907.33	Joback Method
dvisc	0.0000254	Pa×s	983.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382815&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