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

Inchi: InChI=1S/C27H48O4/c1-3-5-7-9-11-12-13-15-19-23-31-27(29)25-21-17-16-20-24(25)26(

InchiKey: WGKYEDRNVLTRBE-UHFFFAOYSA-N

Formula: C27H48O4

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

Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-244.68	kJ/mol	Joback Method
hf	-998.45	kJ/mol	Joback Method
hfus	65.39	kJ/mol	Joback Method
hvap	94.42	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.546		Crippen Method
mcvol	391.010	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	983.78	K	Joback Method
tc	1206.49	K	Joback Method
tf	542.27	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1378.93	J/mol×K	983.78	Joback Method
cpg	1398.60	J/mol×K	1020.90	Joback Method
cpg	1416.38	J/mol×K	1058.02	Joback Method
cpg	1432.34	J/mol×K	1095.13	Joback Method
cpg	1446.51	J/mol×K	1132.25	Joback Method
cpg	1458.95	J/mol×K	1169.37	Joback Method
cpg	1469.72	J/mol×K	1206.49	Joback Method
dvisc	0.0004533	Pa×s	542.27	Joback Method

dvisc	0.0002157	Pa×s	615.86	Joback Method
dvisc	0.0001203	Pa×s	689.44	Joback Method
dvisc	0.0000751	Pa×s	763.03	Joback Method
dvisc	0.0000509	Pa×s	836.61	Joback Method
dvisc	0.0000368	Pa×s	910.20	Joback Method
dvisc	0.0000279	Pa×s	983.78	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=U382756&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

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