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

Inchi: InChI=1S/C27H40O4/c1-2-3-4-5-6-7-8-9-15-21-30-26(28)24-18-13-14-19-25(24)27(29)31

InchiKey: DFTHPDUCEITGAZ-UHFFFAOYSA-N

Formula: C27H40O4

SMILES: CCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 428.60

Physical Properties

Property code	Value	Unit	Source
gf	-132.27	kJ/mol	Joback Method
hf	-761.92	kJ/mol	Joback Method
hfus	59.43	kJ/mol	Joback Method
hvap	96.70	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.429		Crippen Method
mcvol	367.250	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	3128.00		NIST Webbook
rinpol	3128.00		NIST Webbook
tb	1010.46	K	Joback Method
tc	1237.47	K	Joback Method
tf	568.69	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.06	J/mol×K	1010.46	Joback Method
cpg	1290.36	J/mol×K	1048.29	Joback Method
cpg	1304.88	J/mol×K	1086.13	Joback Method
cpg	1317.68	J/mol×K	1123.96	Joback Method
cpg	1328.83	J/mol×K	1161.80	Joback Method
cpg	1338.39	J/mol×K	1199.63	Joback Method
cpg	1346.43	J/mol×K	1237.47	Joback Method
dvisc	0.0003970	Pa×s	568.69	Joback Method

dvisc	0.0001999	Pa×s	642.32	Joback Method
dvisc	0.0001159	Pa×s	715.95	Joback Method
dvisc	0.0000744	Pa×s	789.58	Joback Method
dvisc	0.0000515	Pa×s	863.20	Joback Method
dvisc	0.0000378	Pa×s	936.83	Joback Method
dvisc	0.0000290	Pa×s	1010.46	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U382798&Units=SI

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