cis-Cyclohex-4-en-1,2-dicarboxylic acid, dodecyl isohexyl ester

Inchi: InChI=1S/C26H46O4/c1-4-5-6-7-8-9-10-11-12-15-20-29-25(27)23-18-13-14-19-24(23)26

InchiKey: IAYPLKHNCJZVSJ-UHFFFAOYSA-N

Formula: C26H46O4

SMILES: CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-255.54	kJ/mol	Joback Method
hf	-983.09	kJ/mol	Joback Method
hfus	59.27	kJ/mol	Joback Method
hvap	91.81	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	7.012		Crippen Method
mcvol	376.920	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	2838.00		NIST Webbook
rinpol	2838.00		NIST Webbook
tb	960.46	K	Joback Method
tc	1176.05	K	Joback Method
tf	516.00	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.49	J/mol×K	960.46	Joback Method
cpg	1334.86	J/mol×K	996.39	Joback Method
cpg	1352.46	J/mol×K	1032.32	Joback Method
cpg	1368.34	J/mol×K	1068.26	Joback Method
cpg	1382.55	J/mol×K	1104.19	Joback Method
cpg	1395.13	J/mol×K	1140.12	Joback Method
cpg	1406.12	J/mol×K	1176.05	Joback Method
dvisc	0.0005760	Pa×s	516.00	Joback Method

dvisc	0.0002572	Pa×s	590.08	Joback Method
dvisc	0.0001375	Pa×s	664.15	Joback Method
dvisc	0.0000833	Pa×s	738.23	Joback Method
dvisc	0.0000553	Pa×s	812.31	Joback Method
dvisc	0.0000394	Pa×s	886.38	Joback Method
dvisc	0.0000295	Pa×s	960.46	Joback Method

Sources

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=U382687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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