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

Inchi: InChI=1S/C29H52O4/c1-3-5-7-9-11-13-15-17-21-25-33-29(31)27-23-19-18-22-26(27)28(
InchiKey: GZZYHCOIYZMQRI-UHFFFAOYSA-N
Formula: C29H52O4
SMILES: CCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-227.84	kJ/mol	Joback Method
hf	-1039.73	kJ/mol	Joback Method
hfus	70.57	kJ/mol	Joback Method
hvap	98.87	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.327		Crippen Method
mcvol	419.190	ml/mol	McGowan Method
pc	729.67	kPa	Joback Method
rinpol	3171.00		NIST Webbook
rinpol	3171.00		NIST Webbook
tb	1029.54	K	Joback Method
tc	1269.23	K	Joback Method
tf	564.81	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1507.35	J/mol×K	1029.54	Joback Method
cpg	1587.06	J/mol×K	1229.28	Joback Method
cpg	1575.24	J/mol×K	1189.34	Joback Method
cpg	1561.43	J/mol×K	1149.39	Joback Method
cpg	1545.56	J/mol×K	1109.44	Joback Method
cpg	1527.56	J/mol×K	1069.49	Joback Method
cpg	1596.97	J/mol×K	1269.23	Joback Method
dvisc	0.0000205	Pa×s	1029.54	Joback Method

dvisc	0.0000272	Pa×s	952.08	Joback Method
dvisc	0.0000379	Pa×s	874.63	Joback Method
dvisc	0.0000563	Pa×s	797.17	Joback Method
dvisc	0.0000909	Pa×s	719.72	Joback Method
dvisc	0.0001651	Pa×s	642.26	Joback Method
dvisc	0.0003529	Pa×s	564.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382680&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

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