cis-Cyclohex-4-en-1,2-dicarboxylic acid, hexadecyl hexyl ester

Inchi: InChI=1S/C30H54O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-22-26-34-30(32)28-24-20-

InchiKey: UVCRPGDLOOQUEQ-UHFFFAOYSA-N

Formula: C30H54O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCC

Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-219.42	kJ/mol	Joback Method
hf	-1060.37	kJ/mol	Joback Method
hfus	73.16	kJ/mol	Joback Method
hvap	101.10	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.717		Crippen Method
mcvol	433.280	ml/mol	McGowan Method
pc	693.25	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1052.42	K	Joback Method
tc	1302.58	K	Joback Method
tf	576.08	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1571.89	J/mol×K	1052.42	Joback Method
cpg	1651.29	J/mol×K	1260.89	Joback Method
cpg	1639.88	J/mol×K	1219.19	Joback Method
cpg	1626.32	J/mol×K	1177.50	Joback Method
cpg	1610.52	J/mol×K	1135.81	Joback Method
cpg	1592.41	J/mol×K	1094.11	Joback Method
cpg	1660.66	J/mol×K	1302.58	Joback Method
dvisc	0.0000176	Pa×s	1052.42	Joback Method

dvisc	0.0000233	Pa×s	973.03	Joback Method
dvisc	0.0000326	Pa×s	893.64	Joback Method
dvisc	0.0000485	Pa×s	814.25	Joback Method
dvisc	0.0000788	Pa×s	734.86	Joback Method
dvisc	0.0001439	Pa×s	655.47	Joback Method
dvisc	0.0003102	Pa×s	576.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382672&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

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