cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(decyl) ester

Inchi: InChI=1S/C28H50O4/c1-3-5-7-9-11-13-15-19-23-31-27(29)25-21-17-18-22-26(25)28(30)32-24-20-16-14-12-10-8-6-4-2/h17-18,25-26H,3-16,19-24H2,1-2H3/t25-,26+/m0/s1

InchiKey: OINVPTWRQQEQGR-UHFFFAOYSA-N

Formula: C28H50O4

SMILES: CCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCCCCC

Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-236.26	kJ/mol	Joback Method
hf	-1019.09	kJ/mol	Joback Method
hfus	67.98	kJ/mol	Joback Method
hvap	96.65	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.937		Crippen Method
mcvol	405.100	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	3081.00		NIST Webbook
rinpol	3081.00		NIST Webbook
tb	1006.66	K	Joback Method
tc	1237.24	K	Joback Method
tf	553.54	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1443.01	J/mol×K	1006.66	Joback Method
cpg	1462.94	J/mol×K	1045.09	Joback Method
cpg	1480.83	J/mol×K	1083.52	Joback Method
cpg	1496.76	J/mol×K	1121.95	Joback Method
cpg	1510.76	J/mol×K	1160.38	Joback Method
cpg	1522.92	J/mol×K	1198.81	Joback Method
cpg	1533.29	J/mol×K	1237.24	Joback Method
dvisc	0.0004005	Pa×s	553.54	Joback Method

dvisc	0.0001889	Pa×s	629.06	Joback Method
dvisc	0.0001047	Pa×s	704.58	Joback Method
dvisc	0.0000651	Pa×s	780.10	Joback Method
dvisc	0.0000440	Pa×s	855.62	Joback Method
dvisc	0.0000317	Pa×s	931.14	Joback Method
dvisc	0.0000239	Pa×s	1006.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382679&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