cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-methylpent-3-yl pentadecyl ester

Inchi: InChI=1S/C29H52O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-20-23-32-28(30)25-21-18-19-

InchiKey: HYHXGSKODIMAPX-UHFFFAOYSA-N

Formula: C29H52O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-232.72	kJ/mol	Joback Method
hf	-1050.29	kJ/mol	Joback Method
hfus	63.52	kJ/mol	Joback Method
hvap	98.10	kJ/mol	Joback Method
log10ws	-8.82		Crippen Method
logp	8.181		Crippen Method
mcvol	419.190	ml/mol	McGowan Method
pc	736.02	kPa	Joback Method
rinpol	3142.00		NIST Webbook
rinpol	3142.00		NIST Webbook
tb	1028.66	K	Joback Method
tc	1265.06	K	Joback Method
tf	534.81	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1507.83	J/mol×K	1028.66	Joback Method
cpg	1585.76	J/mol×K	1225.66	Joback Method
cpg	1574.26	J/mol×K	1186.26	Joback Method
cpg	1560.78	J/mol×K	1146.86	Joback Method
cpg	1545.26	J/mol×K	1107.46	Joback Method
cpg	1527.64	J/mol×K	1068.06	Joback Method
cpg	1595.37	J/mol×K	1265.06	Joback Method
dvisc	0.0000170	Pa×s	1028.66	Joback Method

dvisc	0.0000231	Pa×s	946.35	Joback Method
dvisc	0.0000332	Pa×s	864.04	Joback Method
dvisc	0.0000518	Pa×s	781.74	Joback Method
dvisc	0.0000895	Pa×s	699.43	Joback Method
dvisc	0.0001789	Pa×s	617.12	Joback Method
dvisc	0.0004428	Pa×s	534.81	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=U382769&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