1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylcyclohexyl tetradecyl ester

Inchi: InChI=1S/C30H54O4/c1-4-5-6-7-8-9-10-11-12-13-14-17-20-33-29(31)27-18-15-16-19-28

InchiKey: SQUSMZMULYENOK-UHFFFAOYSA-N

Formula: C30H54O4

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1

Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-240.35	kJ/mol	Joback Method
hf	-1104.51	kJ/mol	Joback Method
hfus	65.91	kJ/mol	Joback Method
hvap	100.62	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	8.405		Crippen Method
mcvol	426.720	ml/mol	McGowan Method
pc	732.44	kPa	Joback Method
rinpol	3285.00		NIST Webbook
rinpol	3285.00		NIST Webbook
tb	1063.47	K	Joback Method
tc	1305.38	K	Joback Method
tf	574.22	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1607.10	J/mol×K	1063.47	Joback Method
cpg	1625.65	J/mol×K	1103.79	Joback Method
cpg	1641.47	J/mol×K	1144.11	Joback Method
cpg	1654.63	J/mol×K	1184.43	Joback Method
cpg	1665.18	J/mol×K	1224.74	Joback Method
cpg	1673.18	J/mol×K	1265.06	Joback Method
cpg	1678.70	J/mol×K	1305.38	Joback Method
dvisc	0.0004545	Pa×s	574.22	Joback Method

dvisc	0.0002187	Pa×s	655.76	Joback Method
dvisc	0.0001238	Pa×s	737.30	Joback Method
dvisc	0.0000784	Pa×s	818.85	Joback Method
dvisc	0.0000540	Pa×s	900.39	Joback Method
dvisc	0.0000395	Pa×s	981.93	Joback Method
dvisc	0.0000304	Pa×s	1063.47	Joback Method

Sources

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=U339855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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