1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl undecyl ester

Inchi: InChI=1S/C27H42O4/c1-4-5-6-7-8-9-10-11-14-17-30-26(28)24-15-12-13-16-25(24)27(29

InchiKey: OOBOGMWQKQBIMH-UHFFFAOYSA-N

Formula: C27H42O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-181.49	kJ/mol	Joback Method
hf	-842.64	kJ/mol	Joback Method
hfus	57.43	kJ/mol	Joback Method
hvap	97.73	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.089		Crippen Method
mcvol	371.550	ml/mol	McGowan Method
pc	949.67	kPa	Joback Method
rinpol	3126.00		NIST Webbook
rinpol	3126.00		NIST Webbook
tb	1021.26	K	Joback Method
tc	1250.45	K	Joback Method
tf	592.97	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1304.47	J/mol×K	1021.26	Joback Method
cpg	1320.94	J/mol×K	1059.46	Joback Method
cpg	1335.47	J/mol×K	1097.66	Joback Method
cpg	1348.11	J/mol×K	1135.86	Joback Method
cpg	1358.89	J/mol×K	1174.06	Joback Method
cpg	1367.88	J/mol×K	1212.25	Joback Method
cpg	1375.12	J/mol×K	1250.45	Joback Method
dvisc	0.0003074	Pa×s	592.97	Joback Method

dvisc	0.0001661	Pa×s	664.35	Joback Method
dvisc	0.0001012	Pa×s	735.73	Joback Method
dvisc	0.0000672	Pa×s	807.12	Joback Method
dvisc	0.0000478	Pa×s	878.50	Joback Method
dvisc	0.0000357	Pa×s	949.88	Joback Method
dvisc	0.0000278	Pa×s	1021.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339620&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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