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

Inchi: InChI=1S/C27H48O4/c1-4-5-6-7-8-9-10-11-14-17-30-26(28)24-15-12-13-16-25(24)27(29
InchiKey: PFDGELPEOWUZLU-UHFFFAOYSA-N
Formula: C27H48O4
SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1
Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-265.61	kJ/mol	Joback Method
hf	-1042.59	kJ/mol	Joback Method
hfus	58.14	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	7.235		Crippen Method
mcvol	384.450	ml/mol	McGowan Method
pc	861.50	kPa	Joback Method
rinpol	2971.00		NIST Webbook
rinpol	2971.00		NIST Webbook
tb	994.83	K	Joback Method
tc	1218.12	K	Joback Method
tf	540.41	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1414.64	J/mol×K	994.83	Joback Method
cpg	1433.89	J/mol×K	1032.04	Joback Method
cpg	1450.87	J/mol×K	1069.26	Joback Method
cpg	1465.61	J/mol×K	1106.47	Joback Method
cpg	1478.16	J/mol×K	1143.69	Joback Method
cpg	1488.55	J/mol×K	1180.90	Joback Method
cpg	1496.82	J/mol×K	1218.12	Joback Method
dvisc	0.0006451	Pa×s	540.41	Joback Method

dvisc	0.0003191	Pa×s	616.15	Joback Method
dvisc	0.0001841	Pa×s	691.88	Joback Method
dvisc	0.0001184	Pa×s	767.62	Joback Method
dvisc	0.0000825	Pa×s	843.36	Joback Method
dvisc	0.0000609	Pa×s	919.09	Joback Method
dvisc	0.0000472	Pa×s	994.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339853&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