1,2-Cyclohexanedicarboxylic acid, 2-methylcyclohexyl undecyl ester

Inchi: InChI=1S/C26H46O4/c1-3-4-5-6-7-8-9-10-15-20-29-25(27)22-17-12-13-18-23(22)26(28)3

InchiKey: LLXISYREWPSUIU-UHFFFAOYSA-N

Formula: C26H46O4

SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-266.32	kJ/mol	Joback Method
hf	-1001.61	kJ/mol	Joback Method
hfus	54.48	kJ/mol	Joback Method
hvap	92.02	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.989		Crippen Method
mcvol	370.360	ml/mol	McGowan Method
pc	930.64	kPa	Joback Method
rinpol	2943.00		NIST Webbook
rinpol	2943.00		NIST Webbook
tb	976.62	K	Joback Method
tc	1196.72	K	Joback Method
tf	533.38	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.66	J/mol×K	976.62	Joback Method
cpg	1422.57	J/mol×K	1160.03	Joback Method
cpg	1411.42	J/mol×K	1123.35	Joback Method
cpg	1398.29	J/mol×K	1086.67	Joback Method
cpg	1383.14	J/mol×K	1049.99	Joback Method
cpg	1365.95	J/mol×K	1013.30	Joback Method
cpg	1431.80	J/mol×K	1196.72	Joback Method
dvisc	0.0000407	Pa×s	976.62	Joback Method

dvisc	0.0000534	Pa×s	902.75	Joback Method
dvisc	0.0000736	Pa×s	828.87	Joback Method
dvisc	0.0001080	Pa×s	755.00	Joback Method
dvisc	0.0001723	Pa×s	681.13	Joback Method
dvisc	0.0003077	Pa×s	607.25	Joback Method
dvisc	0.0006456	Pa×s	533.38	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=U339881&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