1,2-Cyclohexanedicarboxylic acid, dodecyl 4-methoxyphenyl ester

Inchi: InChI=1S/C27H42O5/c1-3-4-5-6-7-8-9-10-11-14-21-31-26(28)24-15-12-13-16-25(24)27(2

InchiKey: VSSFWSSBNIUSSY-UHFFFAOYSA-N

Formula: C27H42O5

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(OC)cc1

Mol. weight [g/mol]: 446.62

Physical Properties

Property code	Value	Unit	Source
gf	-276.86	kJ/mol	Joback Method
hf	-963.39	kJ/mol	Joback Method
hfus	59.01	kJ/mol	Joback Method
hvap	99.48	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.871		Crippen Method
mcvol	377.420	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	3334.00		NIST Webbook
rinpol	3334.00		NIST Webbook
tb	1038.70	K	Joback Method
tc	1271.71	K	Joback Method
tf	602.68	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1333.49	J/mol×K	1038.70	Joback Method
cpg	1348.88	J/mol×K	1077.54	Joback Method
cpg	1362.13	J/mol×K	1116.37	Joback Method
cpg	1373.27	J/mol×K	1155.21	Joback Method
cpg	1382.35	J/mol×K	1194.04	Joback Method
cpg	1389.40	J/mol×K	1232.88	Joback Method
cpg	1394.47	J/mol×K	1271.71	Joback Method
dvisc	0.0002399	Pa×s	602.68	Joback Method

dvisc	0.0001268	Pa×s	675.35	Joback Method
dvisc	0.0000759	Pa×s	748.02	Joback Method
dvisc	0.0000497	Pa×s	820.69	Joback Method
dvisc	0.0000349	Pa×s	893.36	Joback Method
dvisc	0.0000258	Pa×s	966.03	Joback Method
dvisc	0.0000200	Pa×s	1038.70	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=U339676&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