1,2-Cyclohexanedicarboxylic acid, undecyl 4-isopropyloxyphenyl diester

Other names: 1,2-Cyclohexanedicarboxylic acid, 4-isopropylphenyl undecyl ester
Inchi: InChI=1S/C28H44O5/c1-4-5-6-7-8-9-10-11-14-21-31-27(29)25-15-12-13-16-26(25)28(30
InchiKey: AZCWAFJFQRQFQS-UHFFFAOYSA-N
Formula: C28H44O5
SMILES: CCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]: 460.65

Physical Properties

Property code	Value	Unit	Source
gf	-270.88	kJ/mol	Joback Method
hf	-989.31	kJ/mol	Joback Method
hfus	58.07	kJ/mol	Joback Method
hvap	101.31	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.260		Crippen Method
mcvol	391.510	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	3177.00		NIST Webbook
rinpol	3177.00		NIST Webbook
tb	1061.14	K	Joback Method
tc	1299.61	K	Joback Method
tf	598.95	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.91	J/mol×K	1061.14	Joback Method
cpg	1449.06	J/mol×K	1259.87	Joback Method
cpg	1442.81	J/mol×K	1220.12	Joback Method
cpg	1434.42	J/mol×K	1180.38	Joback Method
cpg	1423.83	J/mol×K	1140.63	Joback Method
cpg	1411.01	J/mol×K	1100.89	Joback Method
cpg	1453.21	J/mol×K	1299.61	Joback Method

dvisc	0.0000155	Pa×s	1061.14	Joback Method
dvisc	0.0000204	Pa×s	984.11	Joback Method
dvisc	0.0000281	Pa×s	907.08	Joback Method
dvisc	0.0000410	Pa×s	830.04	Joback Method
dvisc	0.0000648	Pa×s	753.01	Joback Method
dvisc	0.0001134	Pa×s	675.98	Joback Method
dvisc	0.0002293	Pa×s	598.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339581&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