1,2-Cyclohexanedicarboxylic acid, dodecyl 2-isopropylphenyl ester

Inchi: InChI=1S/C29H46O4/c1-4-5-6-7-8-9-10-11-12-17-22-32-28(30)25-19-13-14-20-26(25)29

InchiKey: YFYCMVQWJDPEIK-UHFFFAOYSA-N

Formula: C29H46O4

SMILES: CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 458.67

Physical Properties

Property code	Value	Unit	Source
gf	-157.46	kJ/mol	Joback Method
hf	-877.73	kJ/mol	Joback Method
hfus	59.47	kJ/mol	Joback Method
hvap	101.13	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	7.986		Crippen Method
mcvol	399.730	ml/mol	McGowan Method
pc	857.97	kPa	Joback Method
rinpol	3216.00		NIST Webbook
rinpol	3216.00		NIST Webbook
tb	1061.60	K	Joback Method
tc	1300.30	K	Joback Method
tf	587.99	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1431.03	J/mol×K	1061.60	Joback Method
cpg	1492.93	J/mol×K	1260.52	Joback Method
cpg	1484.49	J/mol×K	1220.73	Joback Method
cpg	1474.15	J/mol×K	1180.95	Joback Method
cpg	1461.84	J/mol×K	1141.17	Joback Method
cpg	1447.49	J/mol×K	1101.38	Joback Method
cpg	1499.54	J/mol×K	1300.30	Joback Method
dvisc	0.0000181	Pa×s	1061.60	Joback Method

dvisc	0.0000239	Pa×s	982.66	Joback Method
dvisc	0.0000332	Pa×s	903.73	Joback Method
dvisc	0.0000490	Pa×s	824.79	Joback Method
dvisc	0.0000785	Pa×s	745.86	Joback Method
dvisc	0.0001406	Pa×s	666.92	Joback Method
dvisc	0.0002946	Pa×s	587.99	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=U339706&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