1,2-Cyclohexanedicarboxylic acid, 2-biphenyl nonyl ester

Inchi: InChI=1S/C29H38O4/c1-2-3-4-5-6-7-15-22-32-28(30)25-19-11-12-20-26(25)29(31)33-27

InchiKey: GVYZYXOTSDAQGP-UHFFFAOYSA-N

Formula: C29H38O4

SMILES: CCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1-c1ccccc1

Mol. weight [g/mol]: 450.61

Physical Properties

Property code	Value	Unit	Source
gf	-42.61	kJ/mol	Joback Method
hf	-635.92	kJ/mol	Joback Method
hfus	57.04	kJ/mol	Joback Method
hvap	103.79	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.359		Crippen Method
mcvol	375.970	ml/mol	McGowan Method
pc	1046.65	kPa	Joback Method
rinpol	3287.00		NIST Webbook
rinpol	3287.00		NIST Webbook
tb	1088.72	K	Joback Method
tc	1334.05	K	Joback Method
tf	629.41	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.26	J/mol×K	1088.72	Joback Method
cpg	1365.96	J/mol×K	1293.16	Joback Method
cpg	1360.02	J/mol×K	1252.27	Joback Method
cpg	1352.37	J/mol×K	1211.38	Joback Method
cpg	1342.92	J/mol×K	1170.50	Joback Method
cpg	1331.58	J/mol×K	1129.61	Joback Method
cpg	1370.27	J/mol×K	1334.05	Joback Method
dvisc	0.0000209	Pa×s	1088.72	Joback Method

dvisc	0.0000270	Pa×s	1012.17	Joback Method
dvisc	0.0000363	Pa×s	935.62	Joback Method
dvisc	0.0000515	Pa×s	859.07	Joback Method
dvisc	0.0000782	Pa×s	782.51	Joback Method
dvisc	0.0001300	Pa×s	705.96	Joback Method
dvisc	0.0002446	Pa×s	629.41	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=U339600&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