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

Inchi: InChI=1S/C31H42O4/c1-2-3-4-5-6-7-8-9-17-24-34-30(32)27-21-13-14-22-28(27)31(33)35

InchiKey: NJHQELHSLRFGDE-UHFFFAOYSA-N

Formula: C31H42O4

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

Mol. weight [g/mol]: 478.66

Physical Properties

Property code	Value	Unit	Source
gf	-25.77	kJ/mol	Joback Method
hf	-677.20	kJ/mol	Joback Method
hfus	62.22	kJ/mol	Joback Method
hvap	108.25	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.139		Crippen Method
mcvol	404.150	ml/mol	McGowan Method
pc	927.81	kPa	Joback Method
rinpol	3498.00		NIST Webbook
rinpol	3498.00		NIST Webbook
tb	1134.48	K	Joback Method
tc	1389.14	K	Joback Method
tf	651.95	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.48	J/mol×K	1134.48	Joback Method
cpg	1486.15	J/mol×K	1346.70	Joback Method
cpg	1481.00	J/mol×K	1304.25	Joback Method
cpg	1474.07	J/mol×K	1261.81	Joback Method
cpg	1465.24	J/mol×K	1219.37	Joback Method
cpg	1454.42	J/mol×K	1176.92	Joback Method
cpg	1489.63	J/mol×K	1389.14	Joback Method
dvisc	0.0000154	Pa×s	1134.48	Joback Method

dvisc	0.0000199	Pa×s	1054.06	Joback Method
dvisc	0.0000270	Pa×s	973.64	Joback Method
dvisc	0.0000385	Pa×s	893.22	Joback Method
dvisc	0.0000590	Pa×s	812.79	Joback Method
dvisc	0.0000994	Pa×s	732.37	Joback Method
dvisc	0.0001904	Pa×s	651.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339601&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

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