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

Inchi: InChI=1S/C27H34O4/c1-2-3-4-5-13-20-30-26(28)23-17-9-10-18-24(23)27(29)31-25-19-1

InchiKey: IHVHESCBLJMSJS-UHFFFAOYSA-N

Formula: C27H34O4

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

Mol. weight [g/mol]: 422.56

Physical Properties

Property code	Value	Unit	Source
gf	-59.45	kJ/mol	Joback Method
hf	-594.64	kJ/mol	Joback Method
hfus	51.86	kJ/mol	Joback Method
hvap	99.34	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.579		Crippen Method
mcvol	347.790	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	3082.00		NIST Webbook
rinpol	3082.00		NIST Webbook
tb	1042.96	K	Joback Method
tc	1283.37	K	Joback Method
tf	606.87	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.91	J/mol×K	1042.96	Joback Method
cpg	1209.67	J/mol×K	1083.03	Joback Method
cpg	1221.54	J/mol×K	1123.10	Joback Method
cpg	1231.59	J/mol×K	1163.17	Joback Method
cpg	1239.89	J/mol×K	1203.23	Joback Method
cpg	1246.52	J/mol×K	1243.30	Joback Method
cpg	1251.55	J/mol×K	1283.37	Joback Method
dvisc	0.0003110	Pa×s	606.87	Joback Method

dvisc	0.0001684	Pa×s	679.55	Joback Method
dvisc	0.0001026	Pa×s	752.23	Joback Method
dvisc	0.0000683	Pa×s	824.91	Joback Method
dvisc	0.0000485	Pa×s	897.60	Joback Method
dvisc	0.0000363	Pa×s	970.28	Joback Method
dvisc	0.0000282	Pa×s	1042.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339598&Units=SI

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