1,2-Cyclohexanedicarboxylic acid, di(3-phenylpropyl) ester

Inchi: InChI=1S/C26H32O4/c27-25(29-19-9-15-21-11-3-1-4-12-21)23-17-7-8-18-24(23)26(28)3
InchiKey: LWMUYODOVNQHFB-UHFFFAOYSA-N
Formula: C26H32O4
SMILES: O=C(OCCCc1ccccc1)C1CCCCC1C(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 408.53

Physical Properties

Property code	Value	Unit	Source
gf	-58.24	kJ/mol	Joback Method
hf	-562.53	kJ/mol	Joback Method
hfus	49.66	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.145		Crippen Method
mcvol	333.700	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	3258.00		NIST Webbook
tb	1015.10	K	Joback Method
tc	1253.73	K	Joback Method
tf	583.08	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.31	J/mol×K	1015.10	Joback Method
cpg	1150.54	J/mol×K	1054.87	Joback Method
cpg	1162.94	J/mol×K	1094.64	Joback Method
cpg	1173.59	J/mol×K	1134.41	Joback Method
cpg	1182.56	J/mol×K	1174.18	Joback Method
cpg	1189.95	J/mol×K	1213.96	Joback Method
cpg	1195.81	J/mol×K	1253.73	Joback Method
dvisc	0.0003920	Pa×s	583.08	Joback Method
dvisc	0.0002050	Pa×s	655.08	Joback Method

dvisc	0.0001219	Pa×s	727.09	Joback Method
dvisc	0.0000796	Pa×s	799.09	Joback Method
dvisc	0.0000558	Pa×s	871.09	Joback Method
dvisc	0.0000413	Pa×s	943.10	Joback Method
dvisc	0.0000319	Pa×s	1015.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339501&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