cis-Cyclohex-4-en-1,2-dicarboxylic acid, di(3-phenylpropyl) ester

Inchi: InChI=1S/C26H30O4/c27-25(29-19-9-15-21-11-3-1-4-12-21)23-17-7-8-18-24(23)26(28)3
InchiKey: QEOKOWKFRDBMDS-UHFFFAOYSA-N
Formula: C26H30O4
SMILES: O=C(OCCCc1ccccc1)C1CC=CCC1C(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 406.51

Physical Properties

Property code	Value	Unit	Source
gf	-28.28	kJ/mol	Joback Method
hf	-504.75	kJ/mol	Joback Method
hfus	50.88	kJ/mol	Joback Method
hvap	96.75	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.921		Crippen Method
mcvol	329.400	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		NIST Webbook
tb	1014.26	K	Joback Method
tc	1253.65	K	Joback Method
tf	583.84	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.44	J/mol×K	1014.26	Joback Method
cpg	1118.10	J/mol×K	1054.16	Joback Method
cpg	1130.00	J/mol×K	1094.06	Joback Method
cpg	1140.23	J/mol×K	1133.96	Joback Method
cpg	1148.86	J/mol×K	1173.85	Joback Method
cpg	1155.97	J/mol×K	1213.75	Joback Method
cpg	1161.64	J/mol×K	1253.65	Joback Method
dvisc	0.0003981	Pa×s	583.84	Joback Method

dvisc	0.0002128	Pa×s	655.58	Joback Method
dvisc	0.0001287	Pa×s	727.31	Joback Method
dvisc	0.0000852	Pa×s	799.05	Joback Method
dvisc	0.0000603	Pa×s	870.79	Joback Method
dvisc	0.0000451	Pa×s	942.52	Joback Method
dvisc	0.0000351	Pa×s	1014.26	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=U382786&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