cis-Cyclohex-4-en-1,2-dicarboxylic acid, nonyl 3-phenylpropyl ester

Inchi: InChI=1S/C26H38O4/c1-2-3-4-5-6-7-13-20-29-25(27)23-18-11-12-19-24(23)26(28)30-21

InchiKey: XYNDLRJOKOOZHV-UHFFFAOYSA-N

Formula: C26H38O4

SMILES: CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	-140.69	kJ/mol	Joback Method
hf	-741.28	kJ/mol	Joback Method
hfus	56.84	kJ/mol	Joback Method
hvap	94.47	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.039		Crippen Method
mcvol	353.160	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	3020.00		NIST Webbook
tb	987.58	K	Joback Method
tc	1210.87	K	Joback Method
tf	557.42	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1212.00	J/mol×K	987.58	Joback Method
cpg	1228.33	J/mol×K	1024.80	Joback Method
cpg	1242.94	J/mol×K	1062.01	Joback Method
cpg	1255.91	J/mol×K	1099.23	Joback Method
cpg	1267.28	J/mol×K	1136.44	Joback Method
cpg	1277.10	J/mol×K	1173.66	Joback Method
cpg	1285.45	J/mol×K	1210.87	Joback Method
dvisc	0.0004467	Pa×s	557.42	Joback Method
dvisc	0.0002271	Pa×s	629.11	Joback Method

dvisc	0.0001326	Pa×s	700.81	Joback Method
dvisc	0.0000855	Pa×s	772.50	Joback Method
dvisc	0.0000594	Pa×s	844.19	Joback Method
dvisc	0.0000437	Pa×s	915.89	Joback Method
dvisc	0.0000336	Pa×s	987.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382780&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

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