1,2-Cyclohexanedicarboxylic acid, nonyl 4-isopropyloxyphenyl dieste

Other names: 1,2-Cyclohexanedicarboxylic acid, 4-isopropylphenyl nonyl ester
Inchi: InChI=1S/C26H40O5/c1-4-5-6-7-8-9-12-19-29-25(27)23-13-10-11-14-24(23)26(28)31-22
InchiKey: MTDUZCPRZMIQST-UHFFFAOYSA-N
Formula: C26H40O5
SMILES: CCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]: 432.59

Physical Properties

Property code	Value	Unit	Source
gf	-287.72	kJ/mol	Joback Method
hf	-948.03	kJ/mol	Joback Method
hfus	52.89	kJ/mol	Joback Method
hvap	96.86	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.479		Crippen Method
mcvol	363.330	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	1015.38	K	Joback Method
tc	1243.74	K	Joback Method
tf	576.41	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1271.79	J/mol×K	1015.38	Joback Method
cpg	1287.30	J/mol×K	1053.44	Joback Method
cpg	1300.76	J/mol×K	1091.50	Joback Method
cpg	1312.21	J/mol×K	1129.56	Joback Method
cpg	1321.68	J/mol×K	1167.62	Joback Method
cpg	1329.20	J/mol×K	1205.68	Joback Method
cpg	1334.80	J/mol×K	1243.74	Joback Method

dvisc	0.0002945	Pa×s	576.41	Joback Method
dvisc	0.0001482	Pa×s	649.57	Joback Method
dvisc	0.0000857	Pa×s	722.73	Joback Method
dvisc	0.0000548	Pa×s	795.89	Joback Method
dvisc	0.0000378	Pa×s	869.06	Joback Method
dvisc	0.0000276	Pa×s	942.22	Joback Method
dvisc	0.0000211	Pa×s	1015.38	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=U339580&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