Isophthalic acid, 2-biphenyl nonyl ester

Inchi: InChI=1S/C29H32O4/c1-2-3-4-5-6-7-13-21-32-28(30)24-17-14-18-25(22-24)29(31)33-27
InchiKey: JZVWVYCGZVCITK-UHFFFAOYSA-N
Formula: C29H32O4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1
Mol. weight [g/mol]: 444.56

Physical Properties

Property code	Value	Unit	Source
gf	43.43	kJ/mol	Joback Method
hf	-444.84	kJ/mol	Joback Method
hfus	57.78	kJ/mol	Joback Method
hvap	106.61	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	7.480		Crippen Method
mcvol	363.070	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
rinpol	3534.00		NIST Webbook
tb	1105.50	K	Joback Method
tc	1354.89	K	Joback Method
tf	665.21	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.37	J/mol×K	1105.50	Joback Method
cpg	1218.12	J/mol×K	1147.06	Joback Method
cpg	1228.31	J/mol×K	1188.63	Joback Method
cpg	1237.03	J/mol×K	1230.19	Joback Method
cpg	1244.39	J/mol×K	1271.76	Joback Method
cpg	1250.49	J/mol×K	1313.32	Joback Method
cpg	1255.42	J/mol×K	1354.89	Joback Method
dvisc	0.0001540	Pa×s	665.21	Joback Method
dvisc	0.0000876	Pa×s	738.59	Joback Method

dvisc	0.0000552	Pa×s	811.97	Joback Method
dvisc	0.0000376	Pa×s	885.36	Joback Method
dvisc	0.0000271	Pa×s	958.74	Joback Method
dvisc	0.0000205	Pa×s	1032.12	Joback Method
dvisc	0.0000161	Pa×s	1105.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344564&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