Isophthalic acid, 2-biphenyl hexyl ester

Inchi: InChI=1S/C26H26O4/c1-2-3-4-10-18-29-25(27)21-14-11-15-22(19-21)26(28)30-24-17-9-

InchiKey: WGKHSRDIIIQRBS-UHFFFAOYSA-N

Formula: C26H26O4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1

Mol. weight [g/mol]: 402.48

Physical Properties

Property code	Value	Unit	Source
gf	18.17	kJ/mol	Joback Method
hf	-382.92	kJ/mol	Joback Method
hfus	50.01	kJ/mol	Joback Method
hvap	99.93	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	6.310		Crippen Method
mcvol	320.800	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook
tb	1036.86	K	Joback Method
tc	1281.06	K	Joback Method
tf	631.40	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.16	J/mol×K	1036.86	Joback Method
cpg	1038.00	J/mol×K	1077.56	Joback Method
cpg	1048.33	J/mol×K	1118.26	Joback Method
cpg	1057.25	J/mol×K	1158.96	Joback Method
cpg	1064.82	J/mol×K	1199.66	Joback Method
cpg	1071.13	J/mol×K	1240.36	Joback Method
cpg	1076.26	J/mol×K	1281.06	Joback Method
dvisc	0.0002195	Pa×s	631.40	Joback Method

dvisc	0.0001286	Pa×s	698.98	Joback Method
dvisc	0.0000827	Pa×s	766.55	Joback Method
dvisc	0.0000572	Pa×s	834.13	Joback Method
dvisc	0.0000418	Pa×s	901.71	Joback Method
dvisc	0.0000319	Pa×s	969.28	Joback Method
dvisc	0.0000252	Pa×s	1036.86	Joback Method

Sources

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=U344561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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