Isophthalic acid, 2-biphenyl octyl ester

Inchi: InChI=1S/C28H30O4/c1-2-3-4-5-6-12-20-31-27(29)23-16-13-17-24(21-23)28(30)32-26-1
InchiKey: YVQQBOXQSPIGFS-UHFFFAOYSA-N
Formula: C28H30O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1
Mol. weight [g/mol]: 430.54

Physical Properties

Property code	Value	Unit	Source
gf	35.01	kJ/mol	Joback Method
hf	-424.20	kJ/mol	Joback Method
hfus	55.19	kJ/mol	Joback Method
hvap	104.39	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	7.090		Crippen Method
mcvol	348.980	ml/mol	McGowan Method
pc	1230.28	kPa	Joback Method
rinpol	3426.00		NIST Webbook
rinpol	3426.00		NIST Webbook
tb	1082.62	K	Joback Method
tc	1329.24	K	Joback Method
tf	653.94	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.92	J/mol×K	1082.62	Joback Method
cpg	1190.30	J/mol×K	1288.14	Joback Method
cpg	1184.13	J/mol×K	1247.04	Joback Method
cpg	1176.70	J/mol×K	1205.93	Joback Method
cpg	1167.91	J/mol×K	1164.83	Joback Method
cpg	1157.68	J/mol×K	1123.72	Joback Method
cpg	1195.31	J/mol×K	1329.24	Joback Method
dvisc	0.0000187	Pa×s	1082.62	Joback Method

dvisc	0.0000238	Pa×s	1011.17	Joback Method
dvisc	0.0000314	Pa×s	939.73	Joback Method
dvisc	0.0000433	Pa×s	868.28	Joback Method
dvisc	0.0000633	Pa×s	796.83	Joback Method
dvisc	0.0000998	Pa×s	725.39	Joback Method
dvisc	0.0001738	Pa×s	653.94	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=U344563&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