Isophthalic acid, 2-biphenyl ethyl ester

Inchi: InChI=1S/C22H18O4/c1-2-25-21(23)17-11-8-12-18(15-17)22(24)26-20-14-7-6-13-19(20)
InchiKey: OXWBJNLVOLBYDT-UHFFFAOYSA-N
Formula: C22H18O4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1
Mol. weight [g/mol]: 346.38

Physical Properties

Property code	Value	Unit	Source
gf	-15.51	kJ/mol	Joback Method
hf	-300.36	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	91.03	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	4.749		Crippen Method
mcvol	264.440	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	2803.00		NIST Webbook
rinpol	2803.00		NIST Webbook
tb	945.34	K	Joback Method
tc	1195.68	K	Joback Method
tf	586.32	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.30	J/mol×K	945.34	Joback Method
cpg	837.97	J/mol×K	1153.96	Joback Method
cpg	831.57	J/mol×K	1112.24	Joback Method
cpg	823.87	J/mol×K	1070.51	Joback Method
cpg	814.80	J/mol×K	1028.79	Joback Method
cpg	804.30	J/mol×K	987.06	Joback Method
cpg	843.14	J/mol×K	1195.68	Joback Method
dvisc	0.0000448	Pa×s	945.34	Joback Method

dvisc	0.0000559	Pa×s	885.50	Joback Method
dvisc	0.0000722	Pa×s	825.67	Joback Method
dvisc	0.0000969	Pa×s	765.83	Joback Method
dvisc	0.0001369	Pa×s	705.99	Joback Method
dvisc	0.0002060	Pa×s	646.16	Joback Method
dvisc	0.0003370	Pa×s	586.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344556&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