Isophthalic acid, 2-biphenyl pentyl ester

Inchi: InChI=1S/C25H24O4/c1-2-3-9-17-28-24(26)20-13-10-14-21(18-20)25(27)29-23-16-8-7-1
InchiKey: RXKFPALSYXIHLG-UHFFFAOYSA-N
Formula: C25H24O4
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1
Mol. weight [g/mol]: 388.46

Physical Properties

Property code	Value	Unit	Source
gf	9.75	kJ/mol	Joback Method
hf	-362.28	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	97.71	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	5.920		Crippen Method
mcvol	306.710	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	3119.00		NIST Webbook
rinpol	3119.00		NIST Webbook
tb	1013.98	K	Joback Method
tc	1258.41	K	Joback Method
tf	620.13	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.92	J/mol×K	1013.98	Joback Method
cpg	1012.17	J/mol×K	1217.68	Joback Method
cpg	1005.81	J/mol×K	1176.94	Joback Method
cpg	998.17	J/mol×K	1136.20	Joback Method
cpg	989.20	J/mol×K	1095.46	Joback Method
cpg	978.81	J/mol×K	1054.72	Joback Method
cpg	1017.34	J/mol×K	1258.41	Joback Method
dvisc	0.0000292	Pa×s	1013.98	Joback Method

dvisc	0.0000368	Pa×s	948.34	Joback Method
dvisc	0.0000481	Pa×s	882.70	Joback Method
dvisc	0.0000655	Pa×s	817.06	Joback Method
dvisc	0.0000942	Pa×s	751.41	Joback Method
dvisc	0.0001453	Pa×s	685.77	Joback Method
dvisc	0.0002455	Pa×s	620.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344560&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