Isophthalic acid, 2-biphenyl isobutyl ester

Inchi: InChI=1S/C24H22O4/c1-17(2)16-27-23(25)19-11-8-12-20(15-19)24(26)28-22-14-7-6-13-
InchiKey: BIOANAXMTJUSBT-UHFFFAOYSA-N
Formula: C24H22O4
SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2ccccc2-c2ccccc2)c1
Mol. weight [g/mol]: 374.43

Physical Properties

Property code	Value	Unit	Source
gf	-1.11	kJ/mol	Joback Method
hf	-346.92	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	95.09	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	5.386		Crippen Method
mcvol	292.620	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
tb	990.66	K	Joback Method
tc	1239.00	K	Joback Method
tf	593.86	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.59	J/mol×K	990.66	Joback Method
cpg	920.58	J/mol×K	1032.05	Joback Method
cpg	931.03	J/mol×K	1073.44	Joback Method
cpg	940.01	J/mol×K	1114.83	Joback Method
cpg	947.60	J/mol×K	1156.22	Joback Method
cpg	953.87	J/mol×K	1197.61	Joback Method
cpg	958.89	J/mol×K	1239.00	Joback Method
dvisc	0.0002927	Pa×s	593.86	Joback Method

dvisc	0.0001665	Pa×s	659.99	Joback Method
dvisc	0.0001050	Pa×s	726.13	Joback Method
dvisc	0.0000715	Pa×s	792.26	Joback Method
dvisc	0.0000517	Pa×s	858.39	Joback Method
dvisc	0.0000391	Pa×s	924.53	Joback Method
dvisc	0.0000307	Pa×s	990.66	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=U344558&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