Isophthalic acid, di(1-phenylpropyl) ester

Inchi: InChI=1S/C26H26O4/c1-3-23(19-12-7-5-8-13-19)29-25(27)21-16-11-17-22(18-21)26(28)30-24(4-2)20-14-9-6-10-15-20/h5-18,23-24H,3-4H2,1-2H3

InchiKey: VCOZRJUEVOZDFV-UHFFFAOYSA-N

Formula: C26H26O4

SMILES: CCC(OC(=O)c1cccc(C(=O)OC(CC)c2ccccc2)c1)c1ccccc1

Mol. weight [g/mol]: 402.48

Physical Properties

Property code	Value	Unit	Source
gf	22.92	kJ/mol	Joback Method
hf	-382.01	kJ/mol	Joback Method
hfus	43.36	kJ/mol	Joback Method
hvap	98.50	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	6.303		Crippen Method
mcvol	320.800	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	3157.00		NIST Webbook
tb	1031.00	K	Joback Method
tc	1278.55	K	Joback Method
tf	588.88	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.32	J/mol×K	1031.00	Joback Method
cpg	1074.12	J/mol×K	1237.29	Joback Method
cpg	1067.67	J/mol×K	1196.03	Joback Method
cpg	1059.96	J/mol×K	1154.78	Joback Method
cpg	1050.89	J/mol×K	1113.52	Joback Method
cpg	1040.38	J/mol×K	1072.26	Joback Method
cpg	1079.40	J/mol×K	1278.55	Joback Method
dvisc	0.0000202	Pa×s	1031.00	Joback Method
dvisc	0.0000265	Pa×s	957.31	Joback Method

dvisc	0.0000364	Pa×s	883.63	Joback Method
dvisc	0.0000528	Pa×s	809.94	Joback Method
dvisc	0.0000826	Pa×s	736.25	Joback Method
dvisc	0.0001427	Pa×s	662.57	Joback Method
dvisc	0.0002826	Pa×s	588.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344555&Units=SI

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