Isophthalic acid, heptyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C24H30O5/c1-4-5-6-7-10-16-27-23(25)19-12-11-13-20(17-19)24(26)29-22-15-

InchiKey: ABJNFWZFZDRXBH-UHFFFAOYSA-N

Formula: C24H30O5

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1

Mol. weight [g/mol]: 398.49

Physical Properties

Property code	Value	Unit	Source
gf	-218.52	kJ/mol	Joback Method
hf	-715.67	kJ/mol	Joback Method
hfus	48.46	kJ/mol	Joback Method
hvap	95.23	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	5.820		Crippen Method
mcvol	322.250	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
tb	986.40	K	Joback Method
tc	1213.19	K	Joback Method
tf	589.67	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.46	J/mol×K	986.40	Joback Method
cpg	1056.82	J/mol×K	1024.20	Joback Method
cpg	1068.59	J/mol×K	1062.00	Joback Method
cpg	1078.79	J/mol×K	1099.80	Joback Method
cpg	1087.45	J/mol×K	1137.60	Joback Method
cpg	1094.61	J/mol×K	1175.39	Joback Method
cpg	1100.29	J/mol×K	1213.19	Joback Method
dvisc	0.0002281	Pa×s	589.67	Joback Method

dvisc	0.0001269	Pa×s	655.79	Joback Method
dvisc	0.0000786	Pa×s	721.91	Joback Method
dvisc	0.0000527	Pa×s	788.04	Joback Method
dvisc	0.0000376	Pa×s	854.16	Joback Method
dvisc	0.0000282	Pa×s	920.28	Joback Method
dvisc	0.0000220	Pa×s	986.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344432&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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