Isophthalic acid, isohexyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C27H28O5/c1-20(2)9-8-16-30-26(28)22-11-7-12-23(18-22)27(29)31-19-21-10-

InchiKey: WYHDMCIVGHGCLU-UHFFFAOYSA-N

Formula: C27H28O5

SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1

Mol. weight [g/mol]: 432.51

Physical Properties

Property code	Value	Unit	Source
gf	-80.85	kJ/mol	Joback Method
hf	-541.06	kJ/mol	Joback Method
hfus	50.27	kJ/mol	Joback Method
hvap	104.18	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.429		Crippen Method
mcvol	340.760	ml/mol	McGowan Method
pc	1308.95	kPa	Joback Method
rinpol	3417.00		NIST Webbook
rinpol	3417.00		NIST Webbook
tb	1081.72	K	Joback Method
tc	1329.77	K	Joback Method
tf	649.90	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.38	J/mol×K	1081.72	Joback Method
cpg	1144.40	J/mol×K	1288.43	Joback Method
cpg	1140.88	J/mol×K	1247.09	Joback Method
cpg	1135.79	J/mol×K	1205.74	Joback Method
cpg	1129.05	J/mol×K	1164.40	Joback Method
cpg	1120.60	J/mol×K	1123.06	Joback Method
cpg	1146.40	J/mol×K	1329.77	Joback Method
dvisc	0.0000145	Pa×s	1081.72	Joback Method

dvisc	0.0000186	Pa×s	1009.75	Joback Method
dvisc	0.0000247	Pa×s	937.78	Joback Method
dvisc	0.0000345	Pa×s	865.81	Joback Method
dvisc	0.0000510	Pa×s	793.84	Joback Method
dvisc	0.0000817	Pa×s	721.87	Joback Method
dvisc	0.0001451	Pa×s	649.90	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=U356608&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