Isophthalic acid, hexyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C27H28O5/c1-2-3-4-8-17-30-26(28)22-12-10-13-23(19-22)27(29)31-20-21-11-
InchiKey: PLBCMBRXGNRNJD-UHFFFAOYSA-N
Formula: C27H28O5
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1
Mol. weight [g/mol]: 432.51

Physical Properties

Property code	Value	Unit	Source
gf	-78.41	kJ/mol	Joback Method
hf	-535.78	kJ/mol	Joback Method
hfus	53.79	kJ/mol	Joback Method
hvap	104.57	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.573		Crippen Method
mcvol	340.760	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
rinpol	3460.00		NIST Webbook
tb	1082.16	K	Joback Method
tc	1329.02	K	Joback Method
tf	664.90	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.16	J/mol×K	1082.16	Joback Method
cpg	1120.44	J/mol×K	1123.30	Joback Method
cpg	1128.98	J/mol×K	1164.45	Joback Method
cpg	1135.84	J/mol×K	1205.59	Joback Method
cpg	1141.09	J/mol×K	1246.73	Joback Method
cpg	1144.79	J/mol×K	1287.87	Joback Method
cpg	1147.02	J/mol×K	1329.02	Joback Method
dvisc	0.0001376	Pa×s	664.90	Joback Method
dvisc	0.0000812	Pa×s	734.44	Joback Method

dvisc	0.0000524	Pa×s	803.99	Joback Method
dvisc	0.0000363	Pa×s	873.53	Joback Method
dvisc	0.0000266	Pa×s	943.07	Joback Method
dvisc	0.0000203	Pa×s	1012.62	Joback Method
dvisc	0.0000160	Pa×s	1082.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356609&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

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