Isophthalic acid, pentyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C26H26O5/c1-2-3-7-16-29-25(27)21-11-9-12-22(18-21)26(28)30-19-20-10-8-1
InchiKey: BYJYDCSEQYLEOK-UHFFFAOYSA-N
Formula: C26H26O5
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1
Mol. weight [g/mol]: 418.48

Physical Properties

Property code	Value	Unit	Source
gf	-86.83	kJ/mol	Joback Method
hf	-515.14	kJ/mol	Joback Method
hfus	51.20	kJ/mol	Joback Method
hvap	102.34	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	6.183		Crippen Method
mcvol	326.670	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	3354.00		NIST Webbook
rinpol	3354.00		NIST Webbook
tb	1059.28	K	Joback Method
tc	1304.55	K	Joback Method
tf	653.63	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.84	J/mol×K	1059.28	Joback Method
cpg	1086.52	J/mol×K	1263.67	Joback Method
cpg	1082.55	J/mol×K	1222.79	Joback Method
cpg	1077.06	J/mol×K	1181.91	Joback Method
cpg	1069.99	J/mol×K	1141.04	Joback Method
cpg	1061.26	J/mol×K	1100.16	Joback Method
cpg	1089.01	J/mol×K	1304.55	Joback Method
dvisc	0.0000186	Pa×s	1059.28	Joback Method

dvisc	0.0000235	Pa×s	991.67	Joback Method
dvisc	0.0000307	Pa×s	924.06	Joback Method
dvisc	0.0000418	Pa×s	856.46	Joback Method
dvisc	0.0000600	Pa×s	788.85	Joback Method
dvisc	0.0000922	Pa×s	721.24	Joback Method
dvisc	0.0001549	Pa×s	653.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356607&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