Isophthalic acid, butyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C25H24O5/c1-2-3-15-28-24(26)20-10-8-11-21(17-20)25(27)29-18-19-9-7-14-2
InchiKey: NNMDFRWUXIBCEB-UHFFFAOYSA-N
Formula: C25H24O5
SMILES: CCCCOC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1
Mol. weight [g/mol]: 404.46

Physical Properties

Property code	Value	Unit	Source
gf	-95.25	kJ/mol	Joback Method
hf	-494.50	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	100.12	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.793		Crippen Method
mcvol	312.580	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		NIST Webbook
tb	1036.40	K	Joback Method
tc	1281.07	K	Joback Method
tf	642.36	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.87	J/mol×K	1036.40	Joback Method
cpg	1002.44	J/mol×K	1077.18	Joback Method
cpg	1011.33	J/mol×K	1117.96	Joback Method
cpg	1018.60	J/mol×K	1158.74	Joback Method
cpg	1024.31	J/mol×K	1199.52	Joback Method
cpg	1028.49	J/mol×K	1240.29	Joback Method
cpg	1031.22	J/mol×K	1281.07	Joback Method
dvisc	0.0001738	Pa×s	642.36	Joback Method

dvisc	0.0001046	Pa×s	708.03	Joback Method
dvisc	0.0000686	Pa×s	773.71	Joback Method
dvisc	0.0000480	Pa×s	839.38	Joback Method
dvisc	0.0000354	Pa×s	905.05	Joback Method
dvisc	0.0000272	Pa×s	970.73	Joback Method
dvisc	0.0000216	Pa×s	1036.40	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=U356606&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