Isophthalic acid, isobutyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C25H24O5/c1-18(2)16-28-24(26)20-9-7-10-21(15-20)25(27)29-17-19-8-6-13-2
InchiKey: RSVVXGKBPGURNF-UHFFFAOYSA-N
Formula: C25H24O5
SMILES: CC(C)COC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1
Mol. weight [g/mol]: 404.46

Physical Properties

Property code	Value	Unit	Source
gf	-97.69	kJ/mol	Joback Method
hf	-499.78	kJ/mol	Joback Method
hfus	45.09	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.649		Crippen Method
mcvol	312.580	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	3197.00		NIST Webbook
tb	1035.96	K	Joback Method
tc	1282.66	K	Joback Method
tf	627.36	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.21	J/mol×K	1035.96	Joback Method
cpg	1002.77	J/mol×K	1077.08	Joback Method
cpg	1011.62	J/mol×K	1118.19	Joback Method
cpg	1018.80	J/mol×K	1159.31	Joback Method
cpg	1024.37	J/mol×K	1200.43	Joback Method
cpg	1028.38	J/mol×K	1241.54	Joback Method
cpg	1030.89	J/mol×K	1282.66	Joback Method
dvisc	0.0001841	Pa×s	627.36	Joback Method
dvisc	0.0001056	Pa×s	695.46	Joback Method

dvisc	0.0000669	Pa×s	763.56	Joback Method
dvisc	0.0000457	Pa×s	831.66	Joback Method
dvisc	0.0000331	Pa×s	899.76	Joback Method
dvisc	0.0000250	Pa×s	967.86	Joback Method
dvisc	0.0000197	Pa×s	1035.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356605&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

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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