Phthalic acid, isobutyl 2-methylbenzyl ester

Inchi: InChI=1S/C20H22O4/c1-14(2)12-23-19(21)17-10-6-7-11-18(17)20(22)24-13-16-9-5-4-8-1

InchiKey: YVFZNKVNSDVARJ-UHFFFAOYSA-N

Formula: C20H22O4

SMILES: Cc1ccccc1COC(=O)c1ccccc1C(=O)OCC(C)C

Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-147.20	kJ/mol	Joback Method
hf	-500.89	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.165		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	872.46	K	Joback Method
tc	1099.91	K	Joback Method
tf	522.36	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.90	J/mol×K	872.46	Joback Method
cpg	795.15	J/mol×K	910.37	Joback Method
cpg	808.06	J/mol×K	948.28	Joback Method
cpg	819.68	J/mol×K	986.18	Joback Method
cpg	830.02	J/mol×K	1024.09	Joback Method
cpg	839.13	J/mol×K	1062.00	Joback Method
cpg	847.04	J/mol×K	1099.91	Joback Method
dvisc	0.0004963	Pa×s	522.36	Joback Method

dvisc	0.0002824	Pa×s	580.71	Joback Method
dvisc	0.0001781	Pa×s	639.06	Joback Method
dvisc	0.0001213	Pa×s	697.41	Joback Method
dvisc	0.0000877	Pa×s	755.76	Joback Method
dvisc	0.0000664	Pa×s	814.11	Joback Method
dvisc	0.0000522	Pa×s	872.46	Joback Method

Sources

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=U382849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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