Isophthalic acid, isobutyl 3-phenylpropyl ester

Inchi: InChI=1S/C21H24O4/c1-16(2)15-25-21(23)19-12-6-11-18(14-19)20(22)24-13-7-10-17-8-
InchiKey: XLLNTTQYUFZBFX-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: CC(C)COC(=O)c1cccc(C(=O)OCCCc2ccccc2)c1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-129.15	kJ/mol	Joback Method
hf	-510.06	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	85.48	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.289		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2742.00		NIST Webbook
rinpol	2742.00		NIST Webbook
tb	890.36	K	Joback Method
tc	1115.31	K	Joback Method
tf	521.11	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.84	J/mol×K	890.36	Joback Method
cpg	854.24	J/mol×K	927.85	Joback Method
cpg	867.30	J/mol×K	965.34	Joback Method
cpg	879.07	J/mol×K	1002.83	Joback Method
cpg	889.58	J/mol×K	1040.32	Joback Method
cpg	898.87	J/mol×K	1077.81	Joback Method
cpg	907.00	J/mol×K	1115.31	Joback Method
dvisc	0.0005174	Pa×s	521.11	Joback Method

dvisc	0.0002773	Pa×s	582.65	Joback Method
dvisc	0.0001674	Pa×s	644.19	Joback Method
dvisc	0.0001104	Pa×s	705.73	Joback Method
dvisc	0.0000778	Pa×s	767.28	Joback Method
dvisc	0.0000577	Pa×s	828.82	Joback Method
dvisc	0.0000447	Pa×s	890.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344387&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