Isophthalic acid, isobutyl phenylethyl ester

Inchi: InChI=1S/C20H22O4/c1-15(2)14-24-20(22)18-10-6-9-17(13-18)19(21)23-12-11-16-7-4-3
InchiKey: WFAMPQKQBRXWEV-UHFFFAOYSA-N
Formula: C20H22O4
SMILES: CC(C)COC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-137.57	kJ/mol	Joback Method
hf	-489.42	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	83.25	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	3.899		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	867.48	K	Joback Method
tc	1094.18	K	Joback Method
tf	509.84	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.03	J/mol×K	867.48	Joback Method
cpg	840.94	J/mol×K	1056.40	Joback Method
cpg	831.65	J/mol×K	1018.61	Joback Method
cpg	821.16	J/mol×K	980.83	Joback Method
cpg	809.41	J/mol×K	943.05	Joback Method
cpg	796.39	J/mol×K	905.26	Joback Method
cpg	849.06	J/mol×K	1094.18	Joback Method
dvisc	0.0000514	Pa×s	867.48	Joback Method

dvisc	0.0000662	Pa×s	807.87	Joback Method
dvisc	0.0000889	Pa×s	748.27	Joback Method
dvisc	0.0001255	Pa×s	688.66	Joback Method
dvisc	0.0001892	Pa×s	629.05	Joback Method
dvisc	0.0003108	Pa×s	569.45	Joback Method
dvisc	0.0005734	Pa×s	509.84	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=U344333&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