Isophthalic acid, isobutyl 2-methylphenyl ester

Inchi: InChI=1S/C19H20O4/c1-13(2)12-22-18(20)15-8-6-9-16(11-15)19(21)23-17-10-5-4-7-14(1
InchiKey: JYVHQHVMDWWHFD-UHFFFAOYSA-N
Formula: C19H20O4
SMILES: Cc1ccccc1OC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]: 312.36

Physical Properties

Property code	Value	Unit	Source
gf	-155.62	kJ/mol	Joback Method
hf	-480.25	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	81.69	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.027		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	2470.00		NIST Webbook
tb	849.58	K	Joback Method
tc	1079.45	K	Joback Method
tf	511.09	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.81	J/mol×K	849.58	Joback Method
cpg	737.98	J/mol×K	887.89	Joback Method
cpg	750.83	J/mol×K	926.20	Joback Method
cpg	762.40	J/mol×K	964.51	Joback Method
cpg	772.72	J/mol×K	1002.83	Joback Method
cpg	781.81	J/mol×K	1041.14	Joback Method
cpg	789.70	J/mol×K	1079.45	Joback Method
dvisc	0.0005456	Pa×s	511.09	Joback Method
dvisc	0.0003141	Pa×s	567.50	Joback Method

dvisc	0.0001999	Pa×s	623.92	Joback Method
dvisc	0.0001371	Pa×s	680.34	Joback Method
dvisc	0.0000996	Pa×s	736.75	Joback Method
dvisc	0.0000757	Pa×s	793.16	Joback Method
dvisc	0.0000597	Pa×s	849.58	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=U344346&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