Isophthalic acid, butyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C20H22O6/c1-4-5-12-25-19(21)14-8-6-9-15(13-14)20(22)26-18-16(23-2)10-7-1

InchiKey: MNXJPJLVENTFFS-UHFFFAOYSA-N

Formula: C20H22O6

SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2c(OC)cccc2OC)c1

Mol. weight [g/mol]: 358.39

Physical Properties

Property code	Value	Unit	Source
gf	-364.39	kJ/mol	Joback Method
hf	-771.52	kJ/mol	Joback Method
hfus	42.42	kJ/mol	Joback Method
hvap	89.78	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	3.880		Crippen Method
mcvol	271.760	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2843.00		NIST Webbook
rinpol	2843.00		NIST Webbook
tb	922.72	K	Joback Method
tc	1147.10	K	Joback Method
tf	594.34	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.05	J/mol×K	922.72	Joback Method
cpg	845.45	J/mol×K	960.12	Joback Method
cpg	856.34	J/mol×K	997.51	Joback Method
cpg	865.70	J/mol×K	1034.91	Joback Method
cpg	873.52	J/mol×K	1072.30	Joback Method
cpg	879.80	J/mol×K	1109.70	Joback Method
cpg	884.51	J/mol×K	1147.10	Joback Method
dvisc	0.0002081	Pa×s	594.34	Joback Method

dvisc	0.0001343	Pa×s	649.07	Joback Method
dvisc	0.0000928	Pa×s	703.80	Joback Method
dvisc	0.0000676	Pa×s	758.53	Joback Method
dvisc	0.0000514	Pa×s	813.26	Joback Method
dvisc	0.0000405	Pa×s	867.99	Joback Method
dvisc	0.0000328	Pa×s	922.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344533&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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