Isophthalic acid, 2,6-dimethoxyphenyl ethyl ester

Inchi: InChI=1S/C18H18O6/c1-4-23-17(19)12-7-5-8-13(11-12)18(20)24-16-14(21-2)9-6-10-15(1

InchiKey: KEJUOWFKTLQCGS-UHFFFAOYSA-N

Formula: C18H18O6

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

Mol. weight [g/mol]: 330.33

Physical Properties

Property code	Value	Unit	Source
gf	-381.23	kJ/mol	Joback Method
hf	-730.24	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	85.33	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.100		Crippen Method
mcvol	243.580	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	2653.00		NIST Webbook
rinpol	2653.00		NIST Webbook
tb	876.96	K	Joback Method
tc	1103.73	K	Joback Method
tf	571.80	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.64	J/mol×K	876.96	Joback Method
cpg	766.39	J/mol×K	1065.93	Joback Method
cpg	759.74	J/mol×K	1028.14	Joback Method
cpg	751.62	J/mol×K	990.34	Joback Method
cpg	742.05	J/mol×K	952.55	Joback Method
cpg	731.05	J/mol×K	914.75	Joback Method
cpg	771.55	J/mol×K	1103.73	Joback Method
dvisc	0.0000432	Pa×s	876.96	Joback Method

dvisc	0.0000529	Pa×s	826.10	Joback Method
dvisc	0.0000666	Pa×s	775.24	Joback Method
dvisc	0.0000866	Pa×s	724.38	Joback Method
dvisc	0.0001172	Pa×s	673.52	Joback Method
dvisc	0.0001666	Pa×s	622.66	Joback Method
dvisc	0.0002521	Pa×s	571.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344530&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