Isophthalic acid, ethyl 4-methoxyphenyl ester

Inchi: InChI=1S/C17H16O5/c1-3-21-16(18)12-5-4-6-13(11-12)17(19)22-15-9-7-14(20-2)8-10-15
InchiKey: CEWJHPLJEROCGJ-UHFFFAOYSA-N
Formula: C17H16O5
SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccc(OC)cc2)c1
Mol. weight [g/mol]: 300.31

Physical Properties

Property code	Value	Unit	Source
gf	-275.02	kJ/mol	Joback Method
hf	-565.91	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Joback Method
hvap	80.03	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.091		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	2560.00		NIST Webbook
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tb	826.68	K	Joback Method
tc	1056.95	K	Joback Method
tf	525.78	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.77	J/mol×K	826.68	Joback Method
cpg	650.86	J/mol×K	865.06	Joback Method
cpg	662.68	J/mol×K	903.44	Joback Method
cpg	673.22	J/mol×K	941.82	Joback Method
cpg	682.49	J/mol×K	980.19	Joback Method
cpg	690.50	J/mol×K	1018.57	Joback Method
cpg	697.24	J/mol×K	1056.95	Joback Method
dvisc	0.0004264	Pa×s	525.78	Joback Method

dvisc	0.0002711	Pa×s	575.93	Joback Method
dvisc	0.0001854	Pa×s	626.08	Joback Method
dvisc	0.0001341	Pa×s	676.23	Joback Method
dvisc	0.0001014	Pa×s	726.38	Joback Method
dvisc	0.0000795	Pa×s	776.53	Joback Method
dvisc	0.0000642	Pa×s	826.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344475&Units=SI

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