Isophthalic acid, ethyl 4-formylphenyl ester

Inchi: InChI=1S/C17H14O5/c1-2-21-16(19)13-4-3-5-14(10-13)17(20)22-15-8-6-12(11-18)7-9-15
InchiKey: SMTINYDLPHAULD-UHFFFAOYSA-N
Formula: C17H14O5
SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccc(C=O)cc2)c1
Mol. weight [g/mol]: 298.29

Physical Properties

Property code	Value	Unit	Source
gf	-269.54	kJ/mol	Joback Method
hf	-519.27	kJ/mol	Joback Method
hfus	34.95	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	2.895		Crippen Method
mcvol	219.320	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	852.92	K	Joback Method
tc	1086.95	K	Joback Method
tf	545.55	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.94	J/mol×K	852.92	Joback Method
cpg	633.43	J/mol×K	891.92	Joback Method
cpg	643.72	J/mol×K	930.93	Joback Method
cpg	652.83	J/mol×K	969.93	Joback Method
cpg	660.78	J/mol×K	1008.94	Joback Method
cpg	667.59	J/mol×K	1047.94	Joback Method
cpg	673.29	J/mol×K	1086.95	Joback Method
dvisc	0.0005909	Pa×s	545.55	Joback Method

dvisc	0.0003800	Pa×s	596.78	Joback Method
dvisc	0.0002621	Pa×s	648.01	Joback Method
dvisc	0.0001909	Pa×s	699.24	Joback Method
dvisc	0.0001452	Pa×s	750.46	Joback Method
dvisc	0.0001143	Pa×s	801.69	Joback Method
dvisc	0.0000927	Pa×s	852.92	Joback Method

Sources

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=U344692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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