Isophthalic acid, ethyl 3-methylphenyl ester

Inchi: InChI=1S/C17H16O4/c1-3-20-16(18)13-7-5-8-14(11-13)17(19)21-15-9-4-6-12(2)10-15/h4
InchiKey: OFKGOZKVKPWQAY-UHFFFAOYSA-N
Formula: C17H16O4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2cccc(C)c2)c1
Mol. weight [g/mol]: 284.31

Physical Properties

Property code	Value	Unit	Source
gf	-170.02	kJ/mol	Joback Method
hf	-433.69	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.391		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook
tb	804.26	K	Joback Method
tc	1036.96	K	Joback Method
tf	503.55	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.57	J/mol×K	804.26	Joback Method
cpg	667.89	J/mol×K	998.17	Joback Method
cpg	658.98	J/mol×K	959.39	Joback Method
cpg	648.92	J/mol×K	920.61	Joback Method
cpg	637.67	J/mol×K	881.83	Joback Method
cpg	625.23	J/mol×K	843.04	Joback Method
cpg	675.67	J/mol×K	1036.96	Joback Method
dvisc	0.0000843	Pa×s	804.26	Joback Method

dvisc	0.0001046	Pa×s	754.14	Joback Method
dvisc	0.0001339	Pa×s	704.02	Joback Method
dvisc	0.0001779	Pa×s	653.90	Joback Method
dvisc	0.0002478	Pa×s	603.79	Joback Method
dvisc	0.0003666	Pa×s	553.67	Joback Method
dvisc	0.0005863	Pa×s	503.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344514&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