Isophthalic acid, ethyl phenyl ester

Inchi: InChI=1S/C16H14O4/c1-2-19-15(17)12-7-6-8-13(11-12)16(18)20-14-9-4-3-5-10-14/h3-11
InchiKey: RJLNSBHHLUAXMC-UHFFFAOYSA-N
Formula: C16H14O4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
gf	-168.81	kJ/mol	Joback Method
hf	-401.58	kJ/mol	Joback Method
hfus	30.46	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.083		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	776.40	K	Joback Method
tc	1012.27	K	Joback Method
tf	479.76	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.48	J/mol×K	776.40	Joback Method
cpg	572.01	J/mol×K	815.71	Joback Method
cpg	584.33	J/mol×K	855.02	Joback Method
cpg	595.46	J/mol×K	894.34	Joback Method
cpg	605.44	J/mol×K	933.65	Joback Method
cpg	614.29	J/mol×K	972.96	Joback Method
cpg	622.03	J/mol×K	1012.27	Joback Method
dvisc	0.0007322	Pa×s	479.76	Joback Method

dvisc	0.0004440	Pa×s	529.20	Joback Method
dvisc	0.0002932	Pa×s	578.64	Joback Method
dvisc	0.0002067	Pa×s	628.08	Joback Method
dvisc	0.0001534	Pa×s	677.52	Joback Method
dvisc	0.0001185	Pa×s	726.96	Joback Method
dvisc	0.0000946	Pa×s	776.40	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=U344354&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