Isophthalic acid, ethyl 3-fluorophenyl ester

Inchi: InChI=1S/C16H13FO4/c1-2-20-15(18)11-5-3-6-12(9-11)16(19)21-14-8-4-7-13(17)10-14/h
InchiKey: URUUCSGDGCPBTG-UHFFFAOYSA-N
Formula: C16H13FO4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2cccc(F)c2)c1
Mol. weight [g/mol]: 288.27

Physical Properties

Property code	Value	Unit	Source
gf	-373.25	kJ/mol	Joback Method
hf	-609.16	kJ/mol	Joback Method
hfus	33.15	kJ/mol	Joback Method
hvap	74.58	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.222		Crippen Method
mcvol	205.430	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	780.65	K	Joback Method
tc	1008.11	K	Joback Method
tf	492.87	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.83	J/mol×K	780.65	Joback Method
cpg	577.63	J/mol×K	818.56	Joback Method
cpg	589.32	J/mol×K	856.47	Joback Method
cpg	599.90	J/mol×K	894.38	Joback Method
cpg	609.41	J/mol×K	932.29	Joback Method
cpg	617.85	J/mol×K	970.20	Joback Method
cpg	625.26	J/mol×K	1008.11	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=U344665&Units=SI

Legend

cpg:	Ideal gas heat capacity
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