Isophthalic acid, 3,5-difluorophenyl ethyl ester

Inchi: InChI=1S/C16H12F2O4/c1-2-21-15(19)10-4-3-5-11(6-10)16(20)22-14-8-12(17)7-13(18)9
InchiKey: GBBMJODBYZUDSI-UHFFFAOYSA-N
Formula: C16H12F2O4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1
Mol. weight [g/mol]: 306.26

Physical Properties

Property code	Value	Unit	Source
gf	-577.69	kJ/mol	Joback Method
hf	-816.74	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.361		Crippen Method
mcvol	207.200	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	784.90	K	Joback Method
tc	1004.79	K	Joback Method
tf	505.98	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.14	J/mol×K	784.90	Joback Method
cpg	583.27	J/mol×K	821.55	Joback Method
cpg	594.37	J/mol×K	858.20	Joback Method
cpg	604.45	J/mol×K	894.84	Joback Method
cpg	613.52	J/mol×K	931.49	Joback Method
cpg	621.58	J/mol×K	968.14	Joback Method
cpg	628.66	J/mol×K	1004.79	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=U344367&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