Isophthalic acid, 3,5-difluorophenyl isobutyl ester

Inchi: InChI=1S/C18H16F2O4/c1-11(2)10-23-17(21)12-4-3-5-13(6-12)18(22)24-16-8-14(19)7-1

InchiKey: KUZRLOIEONSDDY-UHFFFAOYSA-N

Formula: C18H16F2O4

SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1

Mol. weight [g/mol]: 334.31

Physical Properties

Property code	Value	Unit	Source
gf	-563.29	kJ/mol	Joback Method
hf	-863.30	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	78.49	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.997		Crippen Method
mcvol	235.380	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	830.22	K	Joback Method
tc	1048.59	K	Joback Method
tf	513.52	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.29	J/mol×K	830.22	Joback Method
cpg	694.12	J/mol×K	866.62	Joback Method
cpg	705.81	J/mol×K	903.01	Joback Method
cpg	716.37	J/mol×K	939.41	Joback Method
cpg	725.83	J/mol×K	975.80	Joback Method
cpg	734.20	J/mol×K	1012.20	Joback Method
cpg	741.49	J/mol×K	1048.59	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=U344369&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