Isophthalic acid, 3,5-difluorophenyl propyl ester

Inchi: InChI=1S/C17H14F2O4/c1-2-6-22-16(20)11-4-3-5-12(7-11)17(21)23-15-9-13(18)8-14(19

InchiKey: BZYGAYUWICITRD-UHFFFAOYSA-N

Formula: C17H14F2O4

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

Mol. weight [g/mol]: 320.29

Physical Properties

Property code	Value	Unit	Source
gf	-569.27	kJ/mol	Joback Method
hf	-837.38	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	3.751		Crippen Method
mcvol	221.290	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	807.78	K	Joback Method
tc	1025.18	K	Joback Method
tf	517.25	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.44	J/mol×K	807.78	Joback Method
cpg	637.88	J/mol×K	844.01	Joback Method
cpg	649.24	J/mol×K	880.25	Joback Method
cpg	659.55	J/mol×K	916.48	Joback Method
cpg	668.82	J/mol×K	952.71	Joback Method
cpg	677.07	J/mol×K	988.95	Joback Method
cpg	684.30	J/mol×K	1025.18	Joback Method

Sources

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=U344368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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