Isophthalic acid, butyl 3,5-difluorophenyl ester

Inchi: InChI=1S/C18H16F2O4/c1-2-3-7-23-17(21)12-5-4-6-13(8-12)18(22)24-16-10-14(19)9-15
InchiKey: FFESEVMTEBJEGH-UHFFFAOYSA-N
Formula: C18H16F2O4
SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1
Mol. weight [g/mol]: 334.31

Physical Properties

Property code	Value	Unit	Source
gf	-560.85	kJ/mol	Joback Method
hf	-858.02	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	78.88	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.141		Crippen Method
mcvol	235.380	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	830.66	K	Joback Method
tc	1046.16	K	Joback Method
tf	528.52	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.71	J/mol×K	830.66	Joback Method
cpg	693.38	J/mol×K	866.58	Joback Method
cpg	704.96	J/mol×K	902.49	Joback Method
cpg	715.45	J/mol×K	938.41	Joback Method
cpg	724.88	J/mol×K	974.33	Joback Method
cpg	733.26	J/mol×K	1010.25	Joback Method
cpg	740.60	J/mol×K	1046.16	Joback Method

Sources

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=U344370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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