Isophthalic acid, 2-bromo-4-fluorophenyl isobutyl ester

Inchi: InChI=1S/C18H16BrFO4/c1-11(2)10-23-17(21)12-4-3-5-13(8-12)18(22)24-16-7-6-14(20)

InchiKey: VDQQAFYESLIENV-UHFFFAOYSA-N

Formula: C18H16BrFO4

SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2ccc(F)cc2Br)c1

Mol. weight [g/mol]: 395.22

Physical Properties

Property code	Value	Unit	Source
gf	-354.16	kJ/mol	Joback Method
hf	-640.86	kJ/mol	Joback Method
hfus	39.71	kJ/mol	Joback Method
hvap	85.74	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.620		Crippen Method
mcvol	251.110	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	897.11	K	Joback Method
tc	1132.09	K	Joback Method
tf	572.73	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.08	J/mol×K	897.11	Joback Method
cpg	717.50	J/mol×K	936.27	Joback Method
cpg	727.71	J/mol×K	975.44	Joback Method
cpg	736.74	J/mol×K	1014.60	Joback Method
cpg	744.64	J/mol×K	1053.76	Joback Method
cpg	751.43	J/mol×K	1092.92	Joback Method
cpg	757.14	J/mol×K	1132.09	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=U344395&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