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

Inchi: InChI=1S/C18H16BrFO4/c1-2-3-9-23-17(21)12-5-4-6-13(10-12)18(22)24-16-8-7-14(20)1

InchiKey: YDGGZSUASKWDAJ-UHFFFAOYSA-N

Formula: C18H16BrFO4

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

Mol. weight [g/mol]: 395.22

Physical Properties

Property code	Value	Unit	Source
gf	-351.72	kJ/mol	Joback Method
hf	-635.58	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	86.13	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	4.764		Crippen Method
mcvol	251.110	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
tb	897.55	K	Joback Method
tc	1129.47	K	Joback Method
tf	587.73	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.53	J/mol×K	897.55	Joback Method
cpg	716.83	J/mol×K	936.20	Joback Method
cpg	726.98	J/mol×K	974.86	Joback Method
cpg	736.00	J/mol×K	1013.51	Joback Method
cpg	743.92	J/mol×K	1052.16	Joback Method
cpg	750.77	J/mol×K	1090.82	Joback Method
cpg	756.59	J/mol×K	1129.47	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=U344396&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