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

Inchi: InChI=1S/C19H18BrFO4/c1-2-3-4-10-24-18(22)13-6-5-7-14(11-13)19(23)25-17-9-8-15(2

InchiKey: VRGOEGONJGYWCG-UHFFFAOYSA-N

Formula: C19H18BrFO4

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

Mol. weight [g/mol]: 409.25

Physical Properties

Property code	Value	Unit	Source
gf	-343.30	kJ/mol	Joback Method
hf	-656.22	kJ/mol	Joback Method
hfus	45.82	kJ/mol	Joback Method
hvap	88.36	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.154		Crippen Method
mcvol	265.200	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	2769.00		NIST Webbook
rinpol	2769.00		NIST Webbook
tb	920.43	K	Joback Method
tc	1150.63	K	Joback Method
tf	599.00	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.09	J/mol×K	920.43	Joback Method
cpg	773.56	J/mol×K	958.80	Joback Method
cpg	783.85	J/mol×K	997.16	Joback Method
cpg	792.99	J/mol×K	1035.53	Joback Method
cpg	801.01	J/mol×K	1073.90	Joback Method
cpg	807.96	J/mol×K	1112.27	Joback Method
cpg	813.85	J/mol×K	1150.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344397&Units=SI
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

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