Phthalic acid, 2-bromo-5-fluorobenzyl isobutyl ester

Inchi: InChI=1S/C19H18BrFO4/c1-12(2)10-24-18(22)15-5-3-4-6-16(15)19(23)25-11-13-9-14(21
InchiKey: MPYWENGUBIOGPW-UHFFFAOYSA-N
Formula: C19H18BrFO4
SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]: 409.25

Physical Properties

Property code	Value	Unit	Source
gf	-345.74	kJ/mol	Joback Method
hf	-661.50	kJ/mol	Joback Method
hfus	42.30	kJ/mol	Joback Method
hvap	87.97	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	4.758		Crippen Method
mcvol	265.200	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
tb	919.99	K	Joback Method
tc	1152.90	K	Joback Method
tf	584.00	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.61	J/mol×K	919.99	Joback Method
cpg	774.18	J/mol×K	958.81	Joback Method
cpg	784.51	J/mol×K	997.63	Joback Method
cpg	793.65	J/mol×K	1036.44	Joback Method
cpg	801.64	J/mol×K	1075.26	Joback Method
cpg	808.51	J/mol×K	1114.08	Joback Method
cpg	814.29	J/mol×K	1152.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382506&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