Phthalic acid, di(2-bromo-5-fluorobenzyl) ester

Inchi: InChI=1S/C22H14Br2F2O4/c23-19-7-5-15(25)9-13(19)11-29-21(27)17-3-1-2-4-18(17)22(
InchiKey: HECCMPHLKXORFU-UHFFFAOYSA-N
Formula: C22H14Br2F2O4
SMILES: O=C(OCc1cc(F)ccc1Br)c1ccccc1C(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]: 540.15

Physical Properties

Property code	Value	Unit	Source
gf	-405.38	kJ/mol	Joback Method
hf	-674.33	kJ/mol	Joback Method
hfus	55.22	kJ/mol	Joback Method
hvap	104.25	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	6.204		Crippen Method
mcvol	302.980	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	3662.00		NIST Webbook
tb	1091.14	K	Joback Method
tc	1349.21	K	Joback Method
tf	744.66	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.12	J/mol×K	1091.14	Joback Method
cpg	857.18	J/mol×K	1134.15	Joback Method
cpg	863.06	J/mol×K	1177.16	Joback Method
cpg	867.81	J/mol×K	1220.18	Joback Method
cpg	871.51	J/mol×K	1263.19	Joback Method
cpg	874.25	J/mol×K	1306.20	Joback Method
cpg	876.08	J/mol×K	1349.21	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=U382518&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