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

Inchi: InChI=1S/C27H34BrFO4/c1-2-3-4-5-6-7-8-9-10-13-18-32-26(30)23-14-11-12-15-24(23)27

InchiKey: ZSRQPWLHQPMADV-UHFFFAOYSA-N

Formula: C27H34BrFO4

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 521.46

Physical Properties

Property code	Value	Unit	Source
gf	-275.94	kJ/mol	Joback Method
hf	-821.34	kJ/mol	Joback Method
hfus	66.54	kJ/mol	Joback Method
hvap	106.16	kJ/mol	Joback Method
log10ws	-10.17		Crippen Method
logp	8.023		Crippen Method
mcvol	377.920	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	3791.00		NIST Webbook
tb	1103.47	K	Joback Method
tc	1351.71	K	Joback Method
tf	689.16	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1235.82	J/mol×K	1103.47	Joback Method
cpg	1248.28	J/mol×K	1144.84	Joback Method
cpg	1259.20	J/mol×K	1186.22	Joback Method
cpg	1268.65	J/mol×K	1227.59	Joback Method
cpg	1276.71	J/mol×K	1268.96	Joback Method
cpg	1283.48	J/mol×K	1310.33	Joback Method
cpg	1289.03	J/mol×K	1351.71	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=U382515&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