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

Inchi: InChI=1S/C26H32BrFO4/c1-2-3-4-5-6-7-8-9-10-11-17-31-25(29)20-13-12-14-21(18-20)2

InchiKey: IVPNSBSFCHWQKQ-UHFFFAOYSA-N

Formula: C26H32BrFO4

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

Mol. weight [g/mol]: 507.43

Physical Properties

Property code	Value	Unit	Source
gf	-284.36	kJ/mol	Joback Method
hf	-800.70	kJ/mol	Joback Method
hfus	63.95	kJ/mol	Joback Method
hvap	103.94	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	7.885		Crippen Method
mcvol	363.830	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
tb	1080.59	K	Joback Method
tc	1322.95	K	Joback Method
tf	677.89	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.98	J/mol×K	1080.59	Joback Method
cpg	1187.30	J/mol×K	1120.98	Joback Method
cpg	1198.14	J/mol×K	1161.38	Joback Method
cpg	1207.57	J/mol×K	1201.77	Joback Method
cpg	1215.68	J/mol×K	1242.17	Joback Method
cpg	1222.52	J/mol×K	1282.56	Joback Method
cpg	1228.19	J/mol×K	1322.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344403&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume