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

Inchi: InChI=1S/C21H22BrFO4/c1-2-3-4-5-6-12-26-20(24)15-8-7-9-16(13-15)21(25)27-19-11-1

InchiKey: KDEINSDNIWUAEG-UHFFFAOYSA-N

Formula: C21H22BrFO4

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

Mol. weight [g/mol]: 437.30

Physical Properties

Property code	Value	Unit	Source
gf	-326.46	kJ/mol	Joback Method
hf	-697.50	kJ/mol	Joback Method
hfus	51.00	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	5.935		Crippen Method
mcvol	293.380	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2992.00		NIST Webbook
rinpol	2992.00		NIST Webbook
tb	966.19	K	Joback Method
tc	1195.30	K	Joback Method
tf	621.54	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.29	J/mol×K	966.19	Joback Method
cpg	889.03	J/mol×K	1004.38	Joback Method
cpg	899.52	J/mol×K	1042.56	Joback Method
cpg	908.82	J/mol×K	1080.75	Joback Method
cpg	916.96	J/mol×K	1118.93	Joback Method
cpg	923.98	J/mol×K	1157.12	Joback Method
cpg	929.94	J/mol×K	1195.30	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=U344400&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

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