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

Inchi: InChI=1S/C20H20BrFO4/c1-13(2)5-4-10-25-19(23)14-6-3-7-15(11-14)20(24)26-18-9-8-1

InchiKey: WQVJYPATQKWXFL-UHFFFAOYSA-N

Formula: C20H20BrFO4

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

Mol. weight [g/mol]: 423.27

Physical Properties

Property code	Value	Unit	Source
gf	-337.32	kJ/mol	Joback Method
hf	-682.14	kJ/mol	Joback Method
hfus	44.89	kJ/mol	Joback Method
hvap	90.19	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.400		Crippen Method
mcvol	279.290	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	942.87	K	Joback Method
tc	1174.46	K	Joback Method
tf	595.27	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.86	J/mol×K	942.87	Joback Method
cpg	831.53	J/mol×K	981.47	Joback Method
cpg	841.96	J/mol×K	1020.07	Joback Method
cpg	851.18	J/mol×K	1058.67	Joback Method
cpg	859.22	J/mol×K	1097.26	Joback Method
cpg	866.14	J/mol×K	1135.86	Joback Method
cpg	871.96	J/mol×K	1174.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344398&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