Isophthalic acid, 3-fluorophenyl hexyl ester

Inchi: InChI=1S/C20H21FO4/c1-2-3-4-5-12-24-19(22)15-8-6-9-16(13-15)20(23)25-18-11-7-10-1
InchiKey: VQZQVWVGTUZELI-UHFFFAOYSA-N
Formula: C20H21FO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2cccc(F)c2)c1
Mol. weight [g/mol]: 344.38

Physical Properties

Property code	Value	Unit	Source
gf	-339.57	kJ/mol	Joback Method
hf	-691.72	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.782		Crippen Method
mcvol	261.790	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2638.00		NIST Webbook
tb	872.17	K	Joback Method
tc	1090.48	K	Joback Method
tf	537.95	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.68	J/mol×K	872.17	Joback Method
cpg	801.27	J/mol×K	908.56	Joback Method
cpg	813.65	J/mol×K	944.94	Joback Method
cpg	824.84	J/mol×K	981.33	Joback Method
cpg	834.86	J/mol×K	1017.71	Joback Method
cpg	843.76	J/mol×K	1054.10	Joback Method
cpg	851.56	J/mol×K	1090.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R474596&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