Phthalic acid, butyl 2-(2-fluorophenyl)ethyl ester

Inchi: InChI=1S/C20H21FO4/c1-2-3-13-24-19(22)16-9-5-6-10-17(16)20(23)25-14-12-15-8-4-7-1

InchiKey: FIHUVZCPRYTEGS-UHFFFAOYSA-N

Formula: C20H21FO4

SMILES: CCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1F

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	-5.58		Crippen Method
logp	4.182		Crippen Method
mcvol	261.790	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378051&Units=SI

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