Terephthalic acid, butyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C19H19FO5/c1-3-4-11-24-18(21)13-5-7-14(8-6-13)19(22)25-16-10-9-15(20)12

InchiKey: OWPZJHVFZZTKDM-UHFFFAOYSA-N

Formula: C19H19FO5

SMILES: CCCCOC(=O)c1ccc(C(=O)Oc2ccc(F)cc2OC)cc1

Mol. weight [g/mol]: 346.35

Physical Properties

Property code	Value	Unit	Source
gf	-462.62	kJ/mol	Joback Method
hf	-814.77	kJ/mol	Joback Method
hfus	41.72	kJ/mol	Joback Method
hvap	84.33	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.010		Crippen Method
mcvol	253.570	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2763.00		NIST Webbook
tb	876.69	K	Joback Method
tc	1096.42	K	Joback Method
tf	561.43	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.23	J/mol×K	876.69	Joback Method
cpg	768.96	J/mol×K	913.31	Joback Method
cpg	780.41	J/mol×K	949.93	Joback Method
cpg	790.58	J/mol×K	986.56	Joback Method
cpg	799.48	J/mol×K	1023.18	Joback Method
cpg	807.10	J/mol×K	1059.80	Joback Method
cpg	813.47	J/mol×K	1096.42	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=U415830&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