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

Inchi: InChI=1S/C19H19FO5/c1-12(2)11-24-18(21)13-4-6-14(7-5-13)19(22)25-16-9-8-15(20)10

InchiKey: RLHXLJIDMHPWCF-UHFFFAOYSA-N

Formula: C19H19FO5

SMILES: COc1cc(F)ccc1OC(=O)c1ccc(C(=O)OCC(C)C)cc1

Mol. weight [g/mol]: 346.35

Physical Properties

Property code	Value	Unit	Source
gf	-465.06	kJ/mol	Joback Method
hf	-820.05	kJ/mol	Joback Method
hfus	38.20	kJ/mol	Joback Method
hvap	83.94	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.866		Crippen Method
mcvol	253.570	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2652.00		NIST Webbook
tb	876.25	K	Joback Method
tc	1098.58	K	Joback Method
tf	546.43	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.78	J/mol×K	876.25	Joback Method
cpg	769.63	J/mol×K	913.30	Joback Method
cpg	781.16	J/mol×K	950.36	Joback Method
cpg	791.36	J/mol×K	987.41	Joback Method
cpg	800.25	J/mol×K	1024.47	Joback Method
cpg	807.83	J/mol×K	1061.52	Joback Method
cpg	814.10	J/mol×K	1098.58	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=U415829&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