Terephthalic acid, 2-fluorobenzyl isobutyl ester

Inchi: InChI=1S/C19H19FO4/c1-13(2)11-23-18(21)14-7-9-15(10-8-14)19(22)24-12-16-5-3-4-6-1

InchiKey: ADCLOSPNMFLQBY-UHFFFAOYSA-N

Formula: C19H19FO4

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCc2ccccc2F)cc1

Mol. weight [g/mol]: 330.35

Physical Properties

Property code	Value	Unit	Source
gf	-350.43	kJ/mol	Joback Method
hf	-676.36	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	3.995		Crippen Method
mcvol	247.700	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2832.00		NIST Webbook
rinpol	2832.00		NIST Webbook
tb	848.85	K	Joback Method
tc	1071.40	K	Joback Method
tf	511.68	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.23	J/mol×K	848.85	Joback Method
cpg	744.84	J/mol×K	885.94	Joback Method
cpg	757.22	J/mol×K	923.03	Joback Method
cpg	768.38	J/mol×K	960.12	Joback Method
cpg	778.37	J/mol×K	997.22	Joback Method
cpg	787.20	J/mol×K	1034.31	Joback Method
cpg	794.92	J/mol×K	1071.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383011&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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