Terephthalic acid, isobutyl 2-fluorophenethyl ester

Inchi: InChI=1S/C20H21FO4/c1-14(2)13-25-20(23)17-9-7-16(8-10-17)19(22)24-12-11-15-5-3-4

InchiKey: GJFZYHRYUGGCHI-UHFFFAOYSA-N

Formula: C20H21FO4

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCCc2ccccc2F)cc1

Mol. weight [g/mol]: 344.38

Physical Properties

Property code	Value	Unit	Source
gf	-342.01	kJ/mol	Joback Method
hf	-697.00	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	83.10	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.038		Crippen Method
mcvol	261.790	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
tb	871.73	K	Joback Method
tc	1092.61	K	Joback Method
tf	522.95	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.22	J/mol×K	871.73	Joback Method
cpg	801.95	J/mol×K	908.54	Joback Method
cpg	814.42	J/mol×K	945.36	Joback Method
cpg	825.65	J/mol×K	982.17	Joback Method
cpg	835.69	J/mol×K	1018.98	Joback Method
cpg	844.56	J/mol×K	1055.79	Joback Method
cpg	852.30	J/mol×K	1092.61	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=U416133&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