Terephthalic acid, butyl 3-fluorobenzyl ester

Inchi: InChI=1S/C19H19FO4/c1-2-3-11-23-18(21)15-7-9-16(10-8-15)19(22)24-13-14-5-4-6-17(2
InchiKey: AOYOWURTKZZKHE-UHFFFAOYSA-N
Formula: C19H19FO4
SMILES: CCCCOC(=O)c1ccc(C(=O)OCc2cccc(F)c2)cc1
Mol. weight [g/mol]: 330.35

Physical Properties

Property code	Value	Unit	Source
gf	-347.99	kJ/mol	Joback Method
hf	-671.08	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	81.26	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.140		Crippen Method
mcvol	247.700	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	849.29	K	Joback Method
tc	1068.94	K	Joback Method
tf	526.68	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.66	J/mol×K	849.29	Joback Method
cpg	744.12	J/mol×K	885.90	Joback Method
cpg	756.39	J/mol×K	922.51	Joback Method
cpg	767.48	J/mol×K	959.12	Joback Method
cpg	777.44	J/mol×K	995.72	Joback Method
cpg	786.29	J/mol×K	1032.33	Joback Method
cpg	794.06	J/mol×K	1068.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416153&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