Terephthalic acid, isobutyl 2,3,5-trifluorobenzyl ester

Inchi: InChI=1S/C19H17F3O4/c1-11(2)9-25-18(23)12-3-5-13(6-4-12)19(24)26-10-14-7-15(20)8

InchiKey: UQQMYMBPPZPIKJ-UHFFFAOYSA-N

Formula: C19H17F3O4

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCc2cc(F)cc(F)c2F)cc1

Mol. weight [g/mol]: 366.33

Physical Properties

Property code	Value	Unit	Source
gf	-759.31	kJ/mol	Joback Method
hf	-1091.52	kJ/mol	Joback Method
hfus	42.78	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.274		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	857.35	K	Joback Method
tc	1069.18	K	Joback Method
tf	537.90	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.57	J/mol×K	857.35	Joback Method
cpg	756.04	J/mol×K	892.66	Joback Method
cpg	767.39	J/mol×K	927.96	Joback Method
cpg	777.63	J/mol×K	963.27	Joback Method
cpg	786.78	J/mol×K	998.57	Joback Method
cpg	794.86	J/mol×K	1033.88	Joback Method
cpg	801.87	J/mol×K	1069.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416031&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