Terephthalic acid, isobutyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C20H19F3O4/c1-13(2)11-26-18(24)15-5-7-16(8-6-15)19(25)27-12-14-3-9-17(1

InchiKey: CDVWOWSCKBQRHA-UHFFFAOYSA-N

Formula: C20H19F3O4

SMILES: CC(C)COC(=O)c1ccc(C(=O)OCc2ccc(C(F)(F)F)cc2)cc1

Mol. weight [g/mol]: 380.36

Physical Properties

Property code	Value	Unit	Source
gf	-728.79	kJ/mol	Joback Method
hf	-1097.97	kJ/mol	Joback Method
hfus	38.74	kJ/mol	Joback Method
hvap	80.17	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.875		Crippen Method
mcvol	265.330	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2761.00		NIST Webbook
rinpol	2761.00		NIST Webbook
tb	867.04	K	Joback Method
tc	1083.12	K	Joback Method
tf	526.55	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.98	J/mol×K	867.04	Joback Method
cpg	816.95	J/mol×K	903.05	Joback Method
cpg	828.77	J/mol×K	939.07	Joback Method
cpg	839.48	J/mol×K	975.08	Joback Method
cpg	849.14	J/mol×K	1011.10	Joback Method
cpg	857.80	J/mol×K	1047.11	Joback Method
cpg	865.51	J/mol×K	1083.12	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=U383030&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