Terephthalic acid, butyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C18H15F3O4/c1-2-3-10-24-17(22)11-4-6-12(7-5-11)18(23)25-14-9-8-13(19)15

InchiKey: IEDKWUCDFNDVGY-UHFFFAOYSA-N

Formula: C18H15F3O4

SMILES: CCCCOC(=O)c1ccc(C(=O)Oc2ccc(F)c(F)c2F)cc1

Mol. weight [g/mol]: 352.30

Physical Properties

Property code	Value	Unit	Source
gf	-765.29	kJ/mol	Joback Method
hf	-1065.60	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	78.72	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.280		Crippen Method
mcvol	237.150	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	834.91	K	Joback Method
tc	1045.07	K	Joback Method
tf	541.63	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.90	J/mol×K	834.91	Joback Method
cpg	699.03	J/mol×K	869.94	Joback Method
cpg	710.11	J/mol×K	904.96	Joback Method
cpg	720.16	J/mol×K	939.99	Joback Method
cpg	729.18	J/mol×K	975.02	Joback Method
cpg	737.20	J/mol×K	1010.04	Joback Method
cpg	744.21	J/mol×K	1045.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415800&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