Terephthalic acid, ethyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C18H15F3O5/c1-2-24-16(22)13-5-7-14(8-6-13)17(23)25-11-12-3-9-15(10-4-12

InchiKey: RZPYWUZNBONJMY-UHFFFAOYSA-N

Formula: C18H15F3O5

SMILES: CCOC(=O)c1ccc(C(=O)OCc2ccc(OC(F)(F)F)cc2)cc1

Mol. weight [g/mol]: 368.30

Physical Properties

Property code	Value	Unit	Source
gf	-848.19	kJ/mol	Joback Method
hf	-1183.63	kJ/mol	Joback Method
hfus	38.27	kJ/mol	Joback Method
hvap	78.51	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.119		Crippen Method
mcvol	243.020	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	844.14	K	Joback Method
tc	1059.40	K	Joback Method
tf	541.24	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.30	J/mol×K	844.14	Joback Method
cpg	729.23	J/mol×K	880.02	Joback Method
cpg	740.03	J/mol×K	915.89	Joback Method
cpg	749.72	J/mol×K	951.77	Joback Method
cpg	758.33	J/mol×K	987.64	Joback Method
cpg	765.89	J/mol×K	1023.52	Joback Method
cpg	772.44	J/mol×K	1059.40	Joback Method

Sources

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=U415973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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