Terephthalic acid, ethyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C12H11F3O4/c1-2-18-10(16)8-3-5-9(6-4-8)11(17)19-7-12(13,14)15/h3-6H,2,7H

InchiKey: XWBHWGYGXXCNBS-UHFFFAOYSA-N

Formula: C12H11F3O4

SMILES: CCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1

Mol. weight [g/mol]: 276.21

Physical Properties

Property code	Value	Unit	Source
gf	-896.49	kJ/mol	Joback Method
hf	-1152.63	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	59.81	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.582		Crippen Method
mcvol	176.370	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook
tb	652.78	K	Joback Method
tc	849.33	K	Joback Method
tf	412.45	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.91	J/mol×K	652.78	Joback Method
cpg	475.93	J/mol×K	685.54	Joback Method
cpg	487.17	J/mol×K	718.30	Joback Method
cpg	497.66	J/mol×K	751.06	Joback Method
cpg	507.40	J/mol×K	783.81	Joback Method
cpg	516.43	J/mol×K	816.57	Joback Method
cpg	524.75	J/mol×K	849.33	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=U383036&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