Terephthalic acid, di(1,1,1-trifluoroprop-2-yl) ester

Inchi: InChI=1S/C14H12F6O4/c1-7(13(15,16)17)23-11(21)9-3-5-10(6-4-9)12(22)24-8(2)14(18,1

InchiKey: YTIGQNXXAYLTFS-UHFFFAOYSA-N

Formula: C14H12F6O4

SMILES: CC(OC(=O)c1ccc(C(=O)OC(C)C(F)(F)F)cc1)C(F)(F)F

Mol. weight [g/mol]: 358.23

Physical Properties

Property code	Value	Unit	Source
gf	-1466.12	kJ/mol	Joback Method
hf	-1801.55	kJ/mol	Joback Method
hfus	27.85	kJ/mol	Joback Method
hvap	59.74	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	3.902		Crippen Method
mcvol	209.860	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
tb	692.24	K	Joback Method
tc	878.77	K	Joback Method
tf	409.18	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.09	J/mol×K	692.24	Joback Method
cpg	606.33	J/mol×K	723.33	Joback Method
cpg	617.71	J/mol×K	754.42	Joback Method
cpg	628.26	J/mol×K	785.51	Joback Method
cpg	638.02	J/mol×K	816.59	Joback Method
cpg	647.03	J/mol×K	847.68	Joback Method
cpg	655.32	J/mol×K	878.77	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=U415772&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