Terephthalic acid, isobutyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C15H17F3O4/c1-9(2)8-21-13(19)11-4-6-12(7-5-11)14(20)22-10(3)15(16,17)18

InchiKey: DXJZXHUILNIGMY-UHFFFAOYSA-N

Formula: C15H17F3O4

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

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-876.11	kJ/mol	Joback Method
hf	-1225.11	kJ/mol	Joback Method
hfus	28.61	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.607		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	720.54	K	Joback Method
tc	917.53	K	Joback Method
tf	416.26	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.64	J/mol×K	720.54	Joback Method
cpg	634.49	J/mol×K	753.37	Joback Method
cpg	647.40	J/mol×K	786.20	Joback Method
cpg	659.40	J/mol×K	819.04	Joback Method
cpg	670.52	J/mol×K	851.87	Joback Method
cpg	680.78	J/mol×K	884.70	Joback Method
cpg	690.21	J/mol×K	917.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415762&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

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