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

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

InchiKey: AWDXPJBKAXOPIY-UHFFFAOYSA-N

Formula: C15H17F3O4

SMILES: CCCCOC(=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	-873.67	kJ/mol	Joback Method
hf	-1219.83	kJ/mol	Joback Method
hfus	32.13	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.751		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
tb	720.98	K	Joback Method
tc	915.14	K	Joback Method
tf	431.26	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.09	J/mol×K	720.98	Joback Method
cpg	633.73	J/mol×K	753.34	Joback Method
cpg	646.46	J/mol×K	785.70	Joback Method
cpg	658.31	J/mol×K	818.06	Joback Method
cpg	669.32	J/mol×K	850.42	Joback Method
cpg	679.50	J/mol×K	882.78	Joback Method
cpg	688.88	J/mol×K	915.14	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=U415763&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