Terephthalic acid, isobutyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C15H15F5O4/c1-9(2)7-23-12(21)10-3-5-11(6-4-10)13(22)24-8-14(16,17)15(18

InchiKey: INMXNBCTWFWDSB-UHFFFAOYSA-N

Formula: C15H15F5O4

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

Mol. weight [g/mol]: 354.27

Physical Properties

Property code	Value	Unit	Source
gf	-1260.45	kJ/mol	Joback Method
hf	-1620.80	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.854		Crippen Method
mcvol	222.180	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	716.29	K	Joback Method
tc	905.39	K	Joback Method
tf	434.86	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.33	J/mol×K	716.29	Joback Method
cpg	651.23	J/mol×K	747.81	Joback Method
cpg	663.23	J/mol×K	779.32	Joback Method
cpg	674.37	J/mol×K	810.84	Joback Method
cpg	684.70	J/mol×K	842.35	Joback Method
cpg	694.25	J/mol×K	873.87	Joback Method
cpg	703.07	J/mol×K	905.39	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=U415789&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