Terephthalic acid, pentyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C21H21F3O4/c1-2-3-7-14-27-19(25)16-10-12-17(13-11-16)20(26)28-18(21(22

InchiKey: JAQVIEYDCLRVKY-UHFFFAOYSA-N

Formula: C21H21F3O4

SMILES: CCCCCOC(=O)c1ccc(C(=O)OC(c2ccccc2)C(F)(F)F)cc1

Mol. weight [g/mol]: 394.38

Physical Properties

Property code	Value	Unit	Source
gf	-710.74	kJ/mol	Joback Method
hf	-1107.14	kJ/mol	Joback Method
hfus	41.72	kJ/mol	Joback Method
hvap	81.73	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.494		Crippen Method
mcvol	279.420	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	884.94	K	Joback Method
tc	1099.74	K	Joback Method
tf	525.30	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.48	J/mol×K	884.94	Joback Method
cpg	875.70	J/mol×K	920.74	Joback Method
cpg	887.75	J/mol×K	956.54	Joback Method
cpg	898.70	J/mol×K	992.34	Joback Method
cpg	908.60	J/mol×K	1028.14	Joback Method
cpg	917.52	J/mol×K	1063.94	Joback Method
cpg	925.51	J/mol×K	1099.74	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415986&Units=SI

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