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

Inchi: InChI=1S/C18H23F3O4/c1-3-4-5-6-7-12-24-16(22)14-8-10-15(11-9-14)17(23)25-13(2)18

InchiKey: BVFIXDOJCZDXIU-UHFFFAOYSA-N

Formula: C18H23F3O4

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

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-848.41	kJ/mol	Joback Method
hf	-1281.75	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	72.78	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.921		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	789.62	K	Joback Method
tc	982.21	K	Joback Method
tf	465.07	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.08	J/mol×K	789.62	Joback Method
cpg	800.67	J/mol×K	821.72	Joback Method
cpg	814.28	J/mol×K	853.82	Joback Method
cpg	826.93	J/mol×K	885.91	Joback Method
cpg	838.66	J/mol×K	918.01	Joback Method
cpg	849.50	J/mol×K	950.11	Joback Method
cpg	859.48	J/mol×K	982.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415766&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