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

Inchi: InChI=1S/C17H21F3O4/c1-3-4-5-6-11-23-15(21)13-7-9-14(10-8-13)16(22)24-12(2)17(18

InchiKey: UYZDGCUGAQKLBA-UHFFFAOYSA-N

Formula: C17H21F3O4

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

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-856.83	kJ/mol	Joback Method
hf	-1261.11	kJ/mol	Joback Method
hfus	37.31	kJ/mol	Joback Method
hvap	70.55	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.531		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2142.00		NIST Webbook
rinpol	2142.00		NIST Webbook
tb	766.74	K	Joback Method
tc	959.29	K	Joback Method
tf	453.80	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.74	J/mol×K	766.74	Joback Method
cpg	744.04	J/mol×K	798.83	Joback Method
cpg	757.38	J/mol×K	830.92	Joback Method
cpg	769.80	J/mol×K	863.02	Joback Method
cpg	781.31	J/mol×K	895.11	Joback Method
cpg	791.96	J/mol×K	927.20	Joback Method
cpg	801.78	J/mol×K	959.29	Joback Method

Sources

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=U415765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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