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

Inchi: InChI=1S/C14H15F3O4/c1-3-8-20-12(18)10-4-6-11(7-5-10)13(19)21-9(2)14(15,16)17/h4-

InchiKey: JJHVLUUDGWVXQI-UHFFFAOYSA-N

Formula: C14H15F3O4

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

Mol. weight [g/mol]: 304.26

Physical Properties

Property code	Value	Unit	Source
gf	-882.09	kJ/mol	Joback Method
hf	-1199.19	kJ/mol	Joback Method
hfus	29.54	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.361		Crippen Method
mcvol	204.550	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	698.10	K	Joback Method
tc	893.80	K	Joback Method
tf	419.99	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.95	J/mol×K	698.10	Joback Method
cpg	580.19	J/mol×K	730.72	Joback Method
cpg	592.55	J/mol×K	763.33	Joback Method
cpg	604.06	J/mol×K	795.95	Joback Method
cpg	614.75	J/mol×K	828.57	Joback Method
cpg	624.63	J/mol×K	861.18	Joback Method
cpg	633.74	J/mol×K	893.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415761&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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