Terephthalic acid, propyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C13H13F3O4/c1-2-7-19-11(17)9-3-5-10(6-4-9)12(18)20-8-13(14,15)16/h3-6H,2

InchiKey: RYGTWOAJGSSVDU-UHFFFAOYSA-N

Formula: C13H13F3O4

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

Mol. weight [g/mol]: 290.24

Physical Properties

Property code	Value	Unit	Source
gf	-888.07	kJ/mol	Joback Method
hf	-1173.27	kJ/mol	Joback Method
hfus	30.48	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.973		Crippen Method
mcvol	190.460	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	675.66	K	Joback Method
tc	870.11	K	Joback Method
tf	423.72	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.50	J/mol×K	675.66	Joback Method
cpg	527.05	J/mol×K	708.07	Joback Method
cpg	538.79	J/mol×K	740.48	Joback Method
cpg	549.75	J/mol×K	772.88	Joback Method
cpg	559.93	J/mol×K	805.29	Joback Method
cpg	569.37	J/mol×K	837.70	Joback Method
cpg	578.08	J/mol×K	870.11	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=U383037&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