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

Inchi: InChI=1S/C19H17F3O4/c1-2-12-25-17(23)14-8-10-15(11-9-14)18(24)26-16(19(20,21)22)

InchiKey: ZGSBYXWVGOCHPZ-UHFFFAOYSA-N

Formula: C19H17F3O4

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

Mol. weight [g/mol]: 366.33

Physical Properties

Property code	Value	Unit	Source
gf	-727.58	kJ/mol	Joback Method
hf	-1065.86	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.714		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	839.18	K	Joback Method
tc	1055.66	K	Joback Method
tf	502.76	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.70	J/mol×K	839.18	Joback Method
cpg	761.60	J/mol×K	875.26	Joback Method
cpg	773.35	J/mol×K	911.34	Joback Method
cpg	784.02	J/mol×K	947.42	Joback Method
cpg	793.65	J/mol×K	983.50	Joback Method
cpg	802.30	J/mol×K	1019.58	Joback Method
cpg	810.03	J/mol×K	1055.66	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=U415983&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