Terephthalic acid, ethyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C13H11F5O4/c1-2-21-10(19)8-3-5-9(6-4-8)11(20)22-7-12(14,15)13(16,17)18/h

InchiKey: MJDKKFQAGLKQKV-UHFFFAOYSA-N

Formula: C13H11F5O4

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

Mol. weight [g/mol]: 326.22

Physical Properties

Property code	Value	Unit	Source
gf	-1274.85	kJ/mol	Joback Method
hf	-1574.24	kJ/mol	Joback Method
hfus	29.22	kJ/mol	Joback Method
hvap	59.11	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.218		Crippen Method
mcvol	194.000	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	670.97	K	Joback Method
tc	859.73	K	Joback Method
tf	427.32	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.56	J/mol×K	670.97	Joback Method
cpg	545.43	J/mol×K	702.43	Joback Method
cpg	556.48	J/mol×K	733.89	Joback Method
cpg	566.73	J/mol×K	765.35	Joback Method
cpg	576.23	J/mol×K	796.81	Joback Method
cpg	585.01	J/mol×K	828.27	Joback Method
cpg	593.10	J/mol×K	859.73	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=U415773&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