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

Inchi: InChI=1S/C14H13F5O4/c1-2-7-22-11(20)9-3-5-10(6-4-9)12(21)23-8-13(15,16)14(17,18)1

InchiKey: AOMWBJGKIVQCRD-UHFFFAOYSA-N

Formula: C14H13F5O4

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

Mol. weight [g/mol]: 340.24

Physical Properties

Property code	Value	Unit	Source
gf	-1266.43	kJ/mol	Joback Method
hf	-1594.88	kJ/mol	Joback Method
hfus	31.81	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.608		Crippen Method
mcvol	208.090	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	693.85	K	Joback Method
tc	881.31	K	Joback Method
tf	438.59	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.07	J/mol×K	693.85	Joback Method
cpg	597.38	J/mol×K	725.09	Joback Method
cpg	608.84	J/mol×K	756.34	Joback Method
cpg	619.50	J/mol×K	787.58	Joback Method
cpg	629.38	J/mol×K	818.83	Joback Method
cpg	638.53	J/mol×K	850.07	Joback Method
cpg	646.98	J/mol×K	881.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415774&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