Terephthalic acid, 2,2,3,4,4,4-hexafluorobutyl pentyl ester

Inchi: InChI=1S/C17H18F6O4/c1-2-3-4-9-26-13(24)11-5-7-12(8-6-11)14(25)27-10-16(19,20)15

InchiKey: HFWAMQHOWVOQLB-UHFFFAOYSA-N

Formula: C17H18F6O4

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

Mol. weight [g/mol]: 400.31

Physical Properties

Property code	Value	Unit	Source
gf	-1438.42	kJ/mol	Joback Method
hf	-1858.19	kJ/mol	Joback Method
hfus	39.14	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.726		Crippen Method
mcvol	252.130	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2131.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	761.32	K	Joback Method
tc	945.19	K	Joback Method
tf	457.99	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.78	J/mol×K	761.32	Joback Method
cpg	767.95	J/mol×K	791.97	Joback Method
cpg	780.23	J/mol×K	822.61	Joback Method
cpg	791.65	J/mol×K	853.26	Joback Method
cpg	802.25	J/mol×K	883.90	Joback Method
cpg	812.08	J/mol×K	914.55	Joback Method
cpg	821.17	J/mol×K	945.19	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=U415752&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