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

Inchi: InChI=1S/C18H20F6O4/c1-2-3-4-5-10-27-14(25)12-6-8-13(9-7-12)15(26)28-11-17(20,21)

InchiKey: CARYOMYDKZDRJU-UHFFFAOYSA-N

Formula: C18H20F6O4

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

Mol. weight [g/mol]: 414.34

Physical Properties

Property code	Value	Unit	Source
gf	-1430.00	kJ/mol	Joback Method
hf	-1878.83	kJ/mol	Joback Method
hfus	41.73	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.116		Crippen Method
mcvol	266.220	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	784.20	K	Joback Method
tc	969.19	K	Joback Method
tf	469.26	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.58	J/mol×K	784.20	Joback Method
cpg	824.10	J/mol×K	815.03	Joback Method
cpg	836.70	J/mol×K	845.86	Joback Method
cpg	848.41	J/mol×K	876.69	Joback Method
cpg	859.29	J/mol×K	907.52	Joback Method
cpg	869.37	J/mol×K	938.36	Joback Method
cpg	878.71	J/mol×K	969.19	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=U415753&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