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

Inchi: InChI=1S/C16H16F6O4/c1-2-3-8-25-12(23)10-4-6-11(7-5-10)13(24)26-9-15(18,19)14(17

InchiKey: SCNRQBYHAPARSZ-UHFFFAOYSA-N

Formula: C16H16F6O4

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

Mol. weight [g/mol]: 386.29

Physical Properties

Property code	Value	Unit	Source
gf	-1446.84	kJ/mol	Joback Method
hf	-1837.55	kJ/mol	Joback Method
hfus	36.55	kJ/mol	Joback Method
hvap	64.58	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.336		Crippen Method
mcvol	238.040	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	738.44	K	Joback Method
tc	921.80	K	Joback Method
tf	446.72	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.96	J/mol×K	738.44	Joback Method
cpg	712.78	J/mol×K	769.00	Joback Method
cpg	724.72	J/mol×K	799.56	Joback Method
cpg	735.83	J/mol×K	830.12	Joback Method
cpg	746.14	J/mol×K	860.68	Joback Method
cpg	755.70	J/mol×K	891.24	Joback Method
cpg	764.54	J/mol×K	921.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415751&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