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

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

InchiKey: CQKXHXVUWRISSH-UHFFFAOYSA-N

Formula: C16H16F6O4

SMILES: CC(C)COC(=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	-1449.28	kJ/mol	Joback Method
hf	-1842.83	kJ/mol	Joback Method
hfus	33.03	kJ/mol	Joback Method
hvap	64.19	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.192		Crippen Method
mcvol	238.040	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
tb	738.00	K	Joback Method
tc	923.43	K	Joback Method
tf	431.72	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.51	J/mol×K	738.00	Joback Method
cpg	713.49	J/mol×K	768.90	Joback Method
cpg	725.57	J/mol×K	799.81	Joback Method
cpg	736.78	J/mol×K	830.71	Joback Method
cpg	747.17	J/mol×K	861.62	Joback Method
cpg	756.78	J/mol×K	892.52	Joback Method
cpg	765.65	J/mol×K	923.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415750&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

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