Terephthalic acid, di(2,2,3,4,4,4-hexafluorobutyl) ester

Inchi: InChI=1S/C16H10F12O4/c17-11(15(23,24)25)13(19,20)5-31-9(29)7-1-2-8(4-3-7)10(30)3

InchiKey: ABNIWOUPOFLHEM-UHFFFAOYSA-N

Formula: C16H10F12O4

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

Mol. weight [g/mol]: 494.23

Physical Properties

Property code	Value	Unit	Source
gf	-2612.46	kJ/mol	Joback Method
hf	-3036.99	kJ/mol	Joback Method
hfus	36.68	kJ/mol	Joback Method
hvap	56.70	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.072		Crippen Method
mcvol	248.660	ml/mol	McGowan Method
pc	1280.99	kPa	Joback Method
rinpol	1696.00		NIST Webbook
rinpol	1696.00		NIST Webbook
tb	727.16	K	Joback Method
tc	897.44	K	Joback Method
tf	440.10	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.25	J/mol×K	727.16	Joback Method
cpg	763.35	J/mol×K	755.54	Joback Method
cpg	773.61	J/mol×K	783.92	Joback Method
cpg	783.09	J/mol×K	812.30	Joback Method
cpg	791.84	J/mol×K	840.68	Joback Method
cpg	799.92	J/mol×K	869.06	Joback Method
cpg	807.38	J/mol×K	897.44	Joback Method

Sources

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=U415760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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