Terephthalic acid, 2,2,3,3,4,4,4-heptafluorobutyl heptyl ester

Inchi: InChI=1S/C19H21F7O4/c1-2-3-4-5-6-11-29-15(27)13-7-9-14(10-8-13)16(28)30-12-17(20

InchiKey: CINBXKODVMVBDY-UHFFFAOYSA-N

Formula: C19H21F7O4

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

Mol. weight [g/mol]: 446.36

Physical Properties

Property code	Value	Unit	Source
gf	-1611.11	kJ/mol	Joback Method
hf	-2099.05	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.803		Crippen Method
mcvol	282.080	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	803.56	K	Joback Method
tc	989.27	K	Joback Method
tf	498.54	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.80	J/mol×K	803.56	Joback Method
cpg	889.26	J/mol×K	834.51	Joback Method
cpg	901.80	J/mol×K	865.46	Joback Method
cpg	913.46	J/mol×K	896.41	Joback Method
cpg	924.30	J/mol×K	927.37	Joback Method
cpg	934.40	J/mol×K	958.32	Joback Method
cpg	943.81	J/mol×K	989.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415941&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