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

Inchi: InChI=1S/C22H28F6O4/c1-2-3-4-5-6-7-8-9-14-31-18(29)16-10-12-17(13-11-16)19(30)32

InchiKey: BRQYIOZWLXSXGO-UHFFFAOYSA-N

Formula: C22H28F6O4

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

Mol. weight [g/mol]: 470.45

Physical Properties

Property code	Value	Unit	Source
gf	-1396.32	kJ/mol	Joback Method
hf	-1961.39	kJ/mol	Joback Method
hfus	52.09	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.677		Crippen Method
mcvol	322.580	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinpol	2615.00		NIST Webbook
tb	875.72	K	Joback Method
tc	1072.32	K	Joback Method
tf	514.34	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.28	J/mol×K	875.72	Joback Method
cpg	1057.30	J/mol×K	908.49	Joback Method
cpg	1071.23	J/mol×K	941.25	Joback Method
cpg	1084.14	J/mol×K	974.02	Joback Method
cpg	1096.10	J/mol×K	1006.78	Joback Method
cpg	1107.16	J/mol×K	1039.55	Joback Method
cpg	1117.40	J/mol×K	1072.32	Joback Method

Sources

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=U415757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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