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

Inchi: InChI=1S/C24H32F6O4/c1-2-3-4-5-6-7-8-9-10-11-16-33-20(31)18-12-14-19(15-13-18)21

InchiKey: PWOLXEJVGFVYJK-UHFFFAOYSA-N

Formula: C24H32F6O4

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

Mol. weight [g/mol]: 498.50

Physical Properties

Property code	Value	Unit	Source
gf	-1379.48	kJ/mol	Joback Method
hf	-2002.67	kJ/mol	Joback Method
hfus	57.27	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.457		Crippen Method
mcvol	350.760	ml/mol	McGowan Method
pc	897.49	kPa	Joback Method
rinpol	1642.00		NIST Webbook
tb	921.48	K	Joback Method
tc	1129.07	K	Joback Method
tf	536.88	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.45	J/mol×K	921.48	Joback Method
cpg	1178.38	J/mol×K	956.08	Joback Method
cpg	1193.11	J/mol×K	990.68	Joback Method
cpg	1206.72	J/mol×K	1025.28	Joback Method
cpg	1219.28	J/mol×K	1059.87	Joback Method
cpg	1230.89	J/mol×K	1094.47	Joback Method
cpg	1241.62	J/mol×K	1129.07	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=U415759&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