Terephthalic acid, dodecyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C23H31F5O4/c1-2-3-4-5-6-7-8-9-10-11-16-31-20(29)18-12-14-19(15-13-18)21

InchiKey: ZQUKKQZMKHBPJB-UHFFFAOYSA-N

Formula: C23H31F5O4

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

Mol. weight [g/mol]: 466.48

Physical Properties

Property code	Value	Unit	Source
gf	-1190.65	kJ/mol	Joback Method
hf	-1780.64	kJ/mol	Joback Method
hfus	55.12	kJ/mol	Joback Method
hvap	81.36	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.119		Crippen Method
mcvol	334.900	ml/mol	McGowan Method
pc	973.52	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
tb	899.77	K	Joback Method
tc	1101.57	K	Joback Method
tf	540.02	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.43	J/mol×K	899.77	Joback Method
cpg	1110.03	J/mol×K	933.40	Joback Method
cpg	1124.51	J/mol×K	967.04	Joback Method
cpg	1137.94	J/mol×K	1000.67	Joback Method
cpg	1150.38	J/mol×K	1034.31	Joback Method
cpg	1161.91	J/mol×K	1067.94	Joback Method
cpg	1172.59	J/mol×K	1101.57	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=U415783&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