Terephthalic acid, dodecyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C23H33F3O4/c1-3-4-5-6-7-8-9-10-11-12-17-29-21(27)19-13-15-20(16-14-19)2

InchiKey: ZZOKNDCIVBIMRZ-UHFFFAOYSA-N

Formula: C23H33F3O4

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

Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
gf	-806.31	kJ/mol	Joback Method
hf	-1384.95	kJ/mol	Joback Method
hfus	52.85	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	6.872		Crippen Method
mcvol	331.360	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
tb	904.02	K	Joback Method
tc	1107.26	K	Joback Method
tf	521.42	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.19	J/mol×K	904.02	Joback Method
cpg	1096.26	J/mol×K	937.89	Joback Method
cpg	1111.12	J/mol×K	971.77	Joback Method
cpg	1124.81	J/mol×K	1005.64	Joback Method
cpg	1137.41	J/mol×K	1039.52	Joback Method
cpg	1148.95	J/mol×K	1073.39	Joback Method
cpg	1159.49	J/mol×K	1107.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415771&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