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

Inchi: InChI=1S/C22H31F3O4/c1-3-4-5-6-7-8-9-10-11-16-28-20(26)18-12-14-19(15-13-18)21(2

InchiKey: UJBDVUOGXCCWGZ-UHFFFAOYSA-N

Formula: C22H31F3O4

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

Mol. weight [g/mol]: 416.47

Physical Properties

Property code	Value	Unit	Source
gf	-814.73	kJ/mol	Joback Method
hf	-1364.31	kJ/mol	Joback Method
hfus	50.26	kJ/mol	Joback Method
hvap	81.68	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.482		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
tb	881.14	K	Joback Method
tc	1080.66	K	Joback Method
tf	510.15	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.93	J/mol×K	881.14	Joback Method
cpg	1035.67	J/mol×K	914.39	Joback Method
cpg	1050.27	J/mol×K	947.65	Joback Method
cpg	1063.76	J/mol×K	980.90	Joback Method
cpg	1076.18	J/mol×K	1014.16	Joback Method
cpg	1087.60	J/mol×K	1047.41	Joback Method
cpg	1098.05	J/mol×K	1080.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415770&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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