Terephthalic acid, hexyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C22H23F3O4/c1-2-3-4-8-15-28-20(26)17-11-13-18(14-12-17)21(27)29-19(22(2

InchiKey: MJUCCCBNGKUQAS-UHFFFAOYSA-N

Formula: C22H23F3O4

SMILES: CCCCCCOC(=O)c1ccc(C(=O)OC(c2ccccc2)C(F)(F)F)cc1

Mol. weight [g/mol]: 408.41

Physical Properties

Property code	Value	Unit	Source
gf	-702.32	kJ/mol	Joback Method
hf	-1127.78	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	83.96	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.884		Crippen Method
mcvol	293.510	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2617.00		NIST Webbook
rinpol	2617.00		NIST Webbook
tb	907.82	K	Joback Method
tc	1122.86	K	Joback Method
tf	536.57	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.47	J/mol×K	907.82	Joback Method
cpg	933.84	J/mol×K	943.66	Joback Method
cpg	946.03	J/mol×K	979.50	Joback Method
cpg	957.10	J/mol×K	1015.34	Joback Method
cpg	967.11	J/mol×K	1051.18	Joback Method
cpg	976.14	J/mol×K	1087.02	Joback Method
cpg	984.24	J/mol×K	1122.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415987&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