Terephthalic acid, di(2,2,2-trifluoro-1-phenylethyl) ester

Inchi: InChI=1S/C24H16F6O4/c25-23(26,27)19(15-7-3-1-4-8-15)33-21(31)17-11-13-18(14-12-1

InchiKey: HSOPHXVPQUPZRD-UHFFFAOYSA-N

Formula: C24H16F6O4

SMILES: O=C(OC(c1ccccc1)C(F)(F)F)c1ccc(C(=O)OC(c2ccccc2)C(F)(F)F)cc1

Mol. weight [g/mol]: 482.37

Physical Properties

Property code	Value	Unit	Source
gf	-1157.10	kJ/mol	Joback Method
hf	-1534.89	kJ/mol	Joback Method
hfus	41.83	kJ/mol	Joback Method
hvap	86.55	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.607		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	974.40	K	Joback Method
tc	1204.38	K	Joback Method
tf	574.72	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.24	J/mol×K	974.40	Joback Method
cpg	963.73	J/mol×K	1012.73	Joback Method
cpg	973.17	J/mol×K	1051.06	Joback Method
cpg	981.69	J/mol×K	1089.39	Joback Method
cpg	989.40	J/mol×K	1127.72	Joback Method
cpg	996.44	J/mol×K	1166.05	Joback Method
cpg	1002.93	J/mol×K	1204.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415990&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