Terephthalic acid, pentyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C21H21F3O5/c1-2-3-4-13-27-19(25)16-7-9-17(10-8-16)20(26)28-14-15-5-11-1

InchiKey: JUKHZDHHAMWVAL-UHFFFAOYSA-N

Formula: C21H21F3O5

SMILES: CCCCCOC(=O)c1ccc(C(=O)OCc2ccc(OC(F)(F)F)cc2)cc1

Mol. weight [g/mol]: 410.38

Physical Properties

Property code	Value	Unit	Source
gf	-822.93	kJ/mol	Joback Method
hf	-1245.55	kJ/mol	Joback Method
hfus	46.04	kJ/mol	Joback Method
hvap	85.19	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.289		Crippen Method
mcvol	285.290	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
tb	912.78	K	Joback Method
tc	1127.40	K	Joback Method
tf	575.05	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.73	J/mol×K	912.78	Joback Method
cpg	900.14	J/mol×K	948.55	Joback Method
cpg	911.31	J/mol×K	984.32	Joback Method
cpg	921.29	J/mol×K	1020.09	Joback Method
cpg	930.11	J/mol×K	1055.86	Joback Method
cpg	937.82	J/mol×K	1091.63	Joback Method
cpg	944.47	J/mol×K	1127.40	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=U415977&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