Terephthalic acid, pentyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C21H21F3O4/c1-2-3-4-13-27-19(25)16-7-9-17(10-8-16)20(26)28-14-15-5-11-1

InchiKey: NRPJYKJWHVKDBE-UHFFFAOYSA-N

Formula: C21H21F3O4

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

Mol. weight [g/mol]: 394.38

Physical Properties

Property code	Value	Unit	Source
gf	-717.93	kJ/mol	Joback Method
hf	-1113.33	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	82.78	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.409		Crippen Method
mcvol	279.420	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2918.00		NIST Webbook
rinpol	2918.00		NIST Webbook
tb	890.36	K	Joback Method
tc	1103.97	K	Joback Method
tf	552.82	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.77	J/mol×K	890.36	Joback Method
cpg	873.80	J/mol×K	925.96	Joback Method
cpg	885.70	J/mol×K	961.56	Joback Method
cpg	896.51	J/mol×K	997.17	Joback Method
cpg	906.29	J/mol×K	1032.77	Joback Method
cpg	915.08	J/mol×K	1068.37	Joback Method
cpg	922.96	J/mol×K	1103.97	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=U383032&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