Terephthalic acid, pentyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C19H17F3O4/c1-2-3-4-11-25-18(23)12-5-7-13(8-6-12)19(24)26-15-10-9-14(20

InchiKey: UGQRYUCIRQOFJE-UHFFFAOYSA-N

Formula: C19H17F3O4

SMILES: CCCCCOC(=O)c1ccc(C(=O)Oc2ccc(F)c(F)c2F)cc1

Mol. weight [g/mol]: 366.33

Physical Properties

Property code	Value	Unit	Source
gf	-756.87	kJ/mol	Joback Method
hf	-1086.24	kJ/mol	Joback Method
hfus	46.31	kJ/mol	Joback Method
hvap	80.95	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	4.670		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
tb	857.79	K	Joback Method
tc	1067.43	K	Joback Method
tf	552.90	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.00	J/mol×K	857.79	Joback Method
cpg	755.37	J/mol×K	892.73	Joback Method
cpg	766.64	J/mol×K	927.67	Joback Method
cpg	776.85	J/mol×K	962.61	Joback Method
cpg	785.99	J/mol×K	997.55	Joback Method
cpg	794.09	J/mol×K	1032.49	Joback Method
cpg	801.16	J/mol×K	1067.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415801&Units=SI

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