Terephthalic acid, 2-fluoro-6-(trifluoromethyl)benzyl propyl ester

Inchi: InChI=1S/C19H16F4O4/c1-2-10-26-17(24)12-6-8-13(9-7-12)18(25)27-11-14-15(19(21,22

InchiKey: DTQSTEKYSSRZKH-UHFFFAOYSA-N

Formula: C19H16F4O4

SMILES: CCCOC(=O)c1ccc(C(=O)OCc2c(F)cccc2C(F)(F)F)cc1

Mol. weight [g/mol]: 384.32

Physical Properties

Property code	Value	Unit	Source
gf	-939.21	kJ/mol	Joback Method
hf	-1279.63	kJ/mol	Joback Method
hfus	42.36	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	4.768		Crippen Method
mcvol	253.010	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
tb	848.85	K	Joback Method
tc	1058.55	K	Joback Method
tf	543.39	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.01	J/mol×K	848.85	Joback Method
cpg	765.15	J/mol×K	883.80	Joback Method
cpg	776.24	J/mol×K	918.75	Joback Method
cpg	786.31	J/mol×K	953.70	Joback Method
cpg	795.42	J/mol×K	988.65	Joback Method
cpg	803.59	J/mol×K	1023.60	Joback Method
cpg	810.88	J/mol×K	1058.55	Joback Method

Sources

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=U382943&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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