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

Inchi: InChI=1S/C21H20F4O4/c1-2-3-4-12-28-19(26)14-8-10-15(11-9-14)20(27)29-13-16-17(21

InchiKey: BNTSHEVYPHYCEQ-UHFFFAOYSA-N

Formula: C21H20F4O4

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

Mol. weight [g/mol]: 412.37

Physical Properties

Property code	Value	Unit	Source
gf	-922.37	kJ/mol	Joback Method
hf	-1320.91	kJ/mol	Joback Method
hfus	47.54	kJ/mol	Joback Method
hvap	82.63	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.549		Crippen Method
mcvol	281.190	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2901.00		NIST Webbook
rinpol	2901.00		NIST Webbook
tb	894.61	K	Joback Method
tc	1104.87	K	Joback Method
tf	565.93	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.81	J/mol×K	894.61	Joback Method
cpg	879.39	J/mol×K	929.65	Joback Method
cpg	890.87	J/mol×K	964.70	Joback Method
cpg	901.28	J/mol×K	999.74	Joback Method
cpg	910.68	J/mol×K	1034.78	Joback Method
cpg	919.11	J/mol×K	1069.82	Joback Method
cpg	926.62	J/mol×K	1104.87	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=U382946&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