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

Inchi: InChI=1S/C25H28F4O4/c1-2-3-4-5-6-7-8-16-32-23(30)18-12-14-19(15-13-18)24(31)33-1

InchiKey: IJEAEWNXFRVNDC-UHFFFAOYSA-N

Formula: C25H28F4O4

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

Mol. weight [g/mol]: 468.48

Physical Properties

Property code	Value	Unit	Source
gf	-888.69	kJ/mol	Joback Method
hf	-1403.47	kJ/mol	Joback Method
hfus	57.90	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	7.109		Crippen Method
mcvol	337.550	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpol	3308.00		NIST Webbook
rinpol	3308.00		NIST Webbook
tb	986.13	K	Joback Method
tc	1207.41	K	Joback Method
tf	611.01	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.50	J/mol×K	986.13	Joback Method
cpg	1115.97	J/mol×K	1023.01	Joback Method
cpg	1128.17	J/mol×K	1059.89	Joback Method
cpg	1139.15	J/mol×K	1096.77	Joback Method
cpg	1148.98	J/mol×K	1133.65	Joback Method
cpg	1157.74	J/mol×K	1170.53	Joback Method
cpg	1165.48	J/mol×K	1207.41	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=U382950&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