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

Inchi: InChI=1S/C26H30F4O4/c1-2-3-4-5-6-7-8-9-17-33-24(31)19-13-15-20(16-14-19)25(32)34

InchiKey: ZOWGNBIAEBSDOG-UHFFFAOYSA-N

Formula: C26H30F4O4

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

Mol. weight [g/mol]: 482.51

Physical Properties

Property code	Value	Unit	Source
gf	-880.27	kJ/mol	Joback Method
hf	-1424.11	kJ/mol	Joback Method
hfus	60.49	kJ/mol	Joback Method
hvap	93.76	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	7.499		Crippen Method
mcvol	351.640	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	3408.00		NIST Webbook
tb	1009.01	K	Joback Method
tc	1235.47	K	Joback Method
tf	622.28	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.80	J/mol×K	1009.01	Joback Method
cpg	1176.54	J/mol×K	1046.75	Joback Method
cpg	1188.94	J/mol×K	1084.50	Joback Method
cpg	1200.07	J/mol×K	1122.24	Joback Method
cpg	1210.00	J/mol×K	1159.98	Joback Method
cpg	1218.82	J/mol×K	1197.73	Joback Method
cpg	1226.61	J/mol×K	1235.47	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=U382951&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