Terephthalic acid, decyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C25H31FO5/c1-3-4-5-6-7-8-9-10-17-30-24(27)19-11-13-20(14-12-19)25(28)31

InchiKey: DRHQWEJKWGPMBZ-UHFFFAOYSA-N

Formula: C25H31FO5

SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)Oc2ccc(F)cc2OC)cc1

Mol. weight [g/mol]: 430.51

Physical Properties

Property code	Value	Unit	Source
gf	-412.10	kJ/mol	Joback Method
hf	-938.61	kJ/mol	Joback Method
hfus	57.26	kJ/mol	Joback Method
hvap	97.69	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.351		Crippen Method
mcvol	338.110	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	2424.00		NIST Webbook
rinpol	2424.00		NIST Webbook
tb	1013.97	K	Joback Method
tc	1241.87	K	Joback Method
tf	629.05	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.72	J/mol×K	1013.97	Joback Method
cpg	1121.66	J/mol×K	1051.95	Joback Method
cpg	1132.94	J/mol×K	1089.94	Joback Method
cpg	1142.60	J/mol×K	1127.92	Joback Method
cpg	1150.66	J/mol×K	1165.90	Joback Method
cpg	1157.15	J/mol×K	1203.88	Joback Method
cpg	1162.11	J/mol×K	1241.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415836&Units=SI
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

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