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

Inchi: InChI=1S/C22H25FO5/c1-3-4-5-6-7-14-27-21(24)16-8-10-17(11-9-16)22(25)28-19-13-12

InchiKey: YMNOTWGTCUHZBA-UHFFFAOYSA-N

Formula: C22H25FO5

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

Mol. weight [g/mol]: 388.43

Physical Properties

Property code	Value	Unit	Source
gf	-437.36	kJ/mol	Joback Method
hf	-876.69	kJ/mol	Joback Method
hfus	49.49	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.181		Crippen Method
mcvol	295.840	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	945.33	K	Joback Method
tc	1165.27	K	Joback Method
tf	595.24	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.05	J/mol×K	945.33	Joback Method
cpg	942.95	J/mol×K	981.99	Joback Method
cpg	954.42	J/mol×K	1018.64	Joback Method
cpg	964.47	J/mol×K	1055.30	Joback Method
cpg	973.13	J/mol×K	1091.95	Joback Method
cpg	980.39	J/mol×K	1128.61	Joback Method
cpg	986.28	J/mol×K	1165.27	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=U415833&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