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

Inchi: InChI=1S/C23H27FO5/c1-3-4-5-6-7-8-15-28-22(25)17-9-11-18(12-10-17)23(26)29-20-14

InchiKey: QRRIUVLCRNOOKN-UHFFFAOYSA-N

Formula: C23H27FO5

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

Mol. weight [g/mol]: 402.46

Physical Properties

Property code	Value	Unit	Source
gf	-428.94	kJ/mol	Joback Method
hf	-897.33	kJ/mol	Joback Method
hfus	52.08	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.571		Crippen Method
mcvol	309.930	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	3182.00		NIST Webbook
rinpol	3182.00		NIST Webbook
tb	968.21	K	Joback Method
tc	1189.86	K	Joback Method
tf	606.51	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.15	J/mol×K	968.21	Joback Method
cpg	1002.07	J/mol×K	1005.15	Joback Method
cpg	1013.50	J/mol×K	1042.09	Joback Method
cpg	1023.45	J/mol×K	1079.04	Joback Method
cpg	1031.94	J/mol×K	1115.98	Joback Method
cpg	1038.99	J/mol×K	1152.92	Joback Method
cpg	1044.62	J/mol×K	1189.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415834&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