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

Inchi: InChI=1S/C24H29FO5/c1-3-4-5-6-7-8-9-16-29-23(26)18-10-12-19(13-11-18)24(27)30-21

InchiKey: FVYPNVIPROLZJW-UHFFFAOYSA-N

Formula: C24H29FO5

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

Mol. weight [g/mol]: 416.48

Physical Properties

Property code	Value	Unit	Source
gf	-420.52	kJ/mol	Joback Method
hf	-917.97	kJ/mol	Joback Method
hfus	54.67	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	5.961		Crippen Method
mcvol	324.020	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinpol	3043.00		NIST Webbook
tb	991.09	K	Joback Method
tc	1215.38	K	Joback Method
tf	617.78	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.72	J/mol×K	991.09	Joback Method
cpg	1061.65	J/mol×K	1028.47	Joback Method
cpg	1073.02	J/mol×K	1065.85	Joback Method
cpg	1082.84	J/mol×K	1103.23	Joback Method
cpg	1091.13	J/mol×K	1140.61	Joback Method
cpg	1097.93	J/mol×K	1178.00	Joback Method
cpg	1103.25	J/mol×K	1215.38	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=U415835&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