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

Inchi: InChI=1S/C17H15FO5/c1-3-22-16(19)11-4-6-12(7-5-11)17(20)23-14-9-8-13(18)10-15(14

InchiKey: QCPQEYVJEAGUKL-UHFFFAOYSA-N

Formula: C17H15FO5

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

Mol. weight [g/mol]: 318.30

Physical Properties

Property code	Value	Unit	Source
gf	-479.46	kJ/mol	Joback Method
hf	-773.49	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.230		Crippen Method
mcvol	225.390	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
tb	830.93	K	Joback Method
tc	1054.15	K	Joback Method
tf	538.89	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.93	J/mol×K	830.93	Joback Method
cpg	656.37	J/mol×K	868.13	Joback Method
cpg	667.62	J/mol×K	905.34	Joback Method
cpg	677.66	J/mol×K	942.54	Joback Method
cpg	686.51	J/mol×K	979.74	Joback Method
cpg	694.14	J/mol×K	1016.95	Joback Method
cpg	700.56	J/mol×K	1054.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415827&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

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