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

Inchi: InChI=1S/C20H21FO5/c1-3-4-5-12-25-19(22)14-6-8-15(9-7-14)20(23)26-17-11-10-16(21

InchiKey: HVUOJSPHCWFURD-UHFFFAOYSA-N

Formula: C20H21FO5

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

Mol. weight [g/mol]: 360.38

Physical Properties

Property code	Value	Unit	Source
gf	-454.20	kJ/mol	Joback Method
hf	-835.41	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	86.56	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.401		Crippen Method
mcvol	267.660	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2871.00		NIST Webbook
rinpol	2871.00		NIST Webbook
tb	899.57	K	Joback Method
tc	1118.60	K	Joback Method
tf	572.70	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.53	J/mol×K	899.57	Joback Method
cpg	826.34	J/mol×K	936.07	Joback Method
cpg	837.82	J/mol×K	972.58	Joback Method
cpg	847.99	J/mol×K	1009.08	Joback Method
cpg	856.85	J/mol×K	1045.59	Joback Method
cpg	864.40	J/mol×K	1082.09	Joback Method
cpg	870.65	J/mol×K	1118.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415831&Units=SI

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