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

Inchi: InChI=1S/C21H23FO5/c1-3-4-5-6-13-26-20(23)15-7-9-16(10-8-15)21(24)27-18-12-11-17

InchiKey: SMMGRRLBOVTRIW-UHFFFAOYSA-N

Formula: C21H23FO5

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

Mol. weight [g/mol]: 374.40

Physical Properties

Property code	Value	Unit	Source
gf	-445.78	kJ/mol	Joback Method
hf	-856.05	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	88.78	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	4.791		Crippen Method
mcvol	281.750	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	2975.00		NIST Webbook
rinpol	2975.00		NIST Webbook
tb	922.45	K	Joback Method
tc	1141.53	K	Joback Method
tf	583.97	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.49	J/mol×K	922.45	Joback Method
cpg	884.36	J/mol×K	958.96	Joback Method
cpg	895.85	J/mol×K	995.48	Joback Method
cpg	905.97	J/mol×K	1031.99	Joback Method
cpg	914.74	J/mol×K	1068.50	Joback Method
cpg	922.17	J/mol×K	1105.02	Joback Method
cpg	928.27	J/mol×K	1141.53	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=U415832&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

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