

Isophthalic acid, 3-fluorophenyl propyl ester

Inchi:	InChI=1S/C17H15FO4/c1-2-9-21-16(19)12-5-3-6-13(10-12)17(20)22-15-8-4-7-14(18)11-
InchiKey:	BVRYVMKHPZFPCK-UHFFFAOYSA-N
Formula:	C17H15FO4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2cccc(F)c2)c1
Mol. weight [g/mol]:	302.30

Physical Properties

Property code	Value	Unit	Source
gf	-364.83	kJ/mol	Joback Method
hf	-629.80	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	76.81	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.612		Crippen Method
mcvol	219.520	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	803.53	K	Joback Method
tc	1027.80	K	Joback Method
tf	504.14	K	Joback Method
vc	0.838	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.17	J/mol×K	803.53	Joback Method
cpg	632.24	J/mol×K	840.91	Joback Method
cpg	644.17	J/mol×K	878.29	Joback Method
cpg	654.97	J/mol×K	915.66	Joback Method
cpg	664.68	J/mol×K	953.04	Joback Method
cpg	673.31	J/mol×K	990.42	Joback Method
cpg	680.88	J/mol×K	1027.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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