Phthalic acid, 3-fluorophenyl isobutyl ester

Inchi: InChI=1S/C18H17FO4/c1-12(2)11-22-17(20)15-8-3-4-9-16(15)18(21)23-14-7-5-6-13(19)1
InchiKey: VBBOWYZLHUVTKQ-UHFFFAOYSA-N
Formula: C18H17FO4
SMILES: CC(C)COC(=O)c1ccccc1C(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 316.32

Physical Properties

Property code	Value	Unit	Source
gf	-358.85	kJ/mol	Joback Method
hf	-655.72	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.858		Crippen Method
mcvol	233.610	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	825.97	K	Joback Method
tc	1050.84	K	Joback Method
tf	500.41	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.05	J/mol×K	825.97	Joback Method
cpg	688.51	J/mol×K	863.45	Joback Method
cpg	700.76	J/mol×K	900.93	Joback Method
cpg	711.82	J/mol×K	938.41	Joback Method
cpg	721.72	J/mol×K	975.89	Joback Method
cpg	730.48	J/mol×K	1013.37	Joback Method
cpg	738.12	J/mol×K	1050.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356497&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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