3-Methoxybenzoic acid, 2,6-difluoro-«alpha»-methylbenzyl ester

Inchi: InChI=1S/C16H14F2O3/c1-10(15-13(17)7-4-8-14(15)18)21-16(19)11-5-3-6-12(9-11)20-2

InchiKey: MAADJJDLWBXDPF-UHFFFAOYSA-N

Formula: C16H14F2O3

SMILES: COc1cccc(C(=O)OC(C)c2c(F)cccc2F)c1

Mol. weight [g/mol]: 292.28

Physical Properties

Property code	Value	Unit	Source
gf	-451.21	kJ/mol	Joback Method
hf	-709.44	kJ/mol	Joback Method
hfus	30.72	kJ/mol	Joback Method
hvap	67.29	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.891		Crippen Method
mcvol	205.630	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	2013.00		NIST Webbook
tb	730.59	K	Joback Method
tc	948.21	K	Joback Method
tf	441.05	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.61	J/mol×K	730.59	Joback Method
cpg	572.73	J/mol×K	766.86	Joback Method
cpg	585.81	J/mol×K	803.13	Joback Method
cpg	597.86	J/mol×K	839.40	Joback Method
cpg	608.91	J/mol×K	875.67	Joback Method
cpg	618.96	J/mol×K	911.94	Joback Method
cpg	628.03	J/mol×K	948.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374930&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

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