

2-Methoxybenzoic acid, 2-fluoro-«alpha»-methylbenzyl ester

Inchi:	InChI=1S/C16H15FO3/c1-11(12-7-3-5-9-14(12)17)20-16(18)13-8-4-6-10-15(13)19-2/h3-
InchiKey:	VSAHPJFCCZRPMM-UHFFFAOYSA-N
Formula:	C16H15FO3
SMILES:	COc1ccccc1C(=O)OC(C)c1ccccc1F
Mol. weight [g/mol]:	274.29

Physical Properties

Property code	Value	Unit	Source
gf	-246.77	kJ/mol	Joback Method
hf	-501.86	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.752		Crippen Method
mcvol	203.860	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinsol	2000.00		NIST Webbook
tb	726.34	K	Joback Method
tc	952.21	K	Joback Method
tf	427.94	K	Joback Method
vc	0.769	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.83	J/mol×K	726.34	Joback Method
cpg	566.75	J/mol×K	763.98	Joback Method
cpg	580.53	J/mol×K	801.63	Joback Method
cpg	593.20	J/mol×K	839.27	Joback Method
cpg	604.78	J/mol×K	876.92	Joback Method
cpg	615.29	J/mol×K	914.56	Joback Method
cpg	624.75	J/mol×K	952.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U374926&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
mccvol:	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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