

4-Methoxybenzoic acid, 2-fluorobenzyl ester

Inchi:	InChI=1S/C15H13FO3/c1-18-13-8-6-11(7-9-13)15(17)19-10-12-4-2-3-5-14(12)16/h2-9H,
InchiKey:	XVAMTJYUNUIRLW-UHFFFAOYSA-N
Formula:	C15H13FO3
SMILES:	COc1ccc(C(=O)OCc2ccccc2F)cc1
Mol. weight [g/mol]:	260.26

Physical Properties

Property code	Value	Unit	Source
gf	-252.75	kJ/mol	Joback Method
hf	-475.94	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.191		Crippen Method
mcvol	189.770	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinsol	2092.00		NIST Webbook
tb	703.90	K	Joback Method
tc	929.52	K	Joback Method
tf	431.67	K	Joback Method
vc	0.720	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.50	J/mol×K	703.90	Joback Method
cpg	512.76	J/mol×K	741.50	Joback Method
cpg	525.96	J/mol×K	779.11	Joback Method
cpg	538.12	J/mol×K	816.71	Joback Method
cpg	549.27	J/mol×K	854.32	Joback Method
cpg	559.41	J/mol×K	891.92	Joback Method
cpg	568.57	J/mol×K	929.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374937&Units=SI
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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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