2-Methoxybenzoic acid, 2-fluorobenzyl ester

Inchi: InChI=1S/C15H13FO3/c1-18-14-9-5-3-7-12(14)15(17)19-10-11-6-2-4-8-13(11)16/h2-9H,1
InchiKey: BVNJJHVNJKLFSJ-UHFFFAOYSA-N
Formula: C15H13FO3
SMILES: COc1ccccc1C(=O)OCc1ccccc1F
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
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
tb	703.90	K	Joback Method
tc	929.52	K	Joback Method
tf	431.67	K	Joback Method
vc	0.720	m3/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

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=U374924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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