4-(Methylthio)benzoic acid, 2-fluorobenzyl ester

Inchi: InChI=1S/C15H13FO2S/c1-19-13-8-6-11(7-9-13)15(17)18-10-12-4-2-3-5-14(12)16/h2-9H

InchiKey: QAPIEUYRPAFCBN-UHFFFAOYSA-N

Formula: C15H13FO2S

SMILES: CSc1ccc(C(=O)OCc2ccccc2F)cc1

Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-114.63	kJ/mol	Joback Method
hf	-301.85	kJ/mol	Joback Method
hfus	31.91	kJ/mol	Joback Method
hvap	70.02	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.905		Crippen Method
mcvol	200.250	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	750.26	K	Joback Method
tc	993.91	K	Joback Method
tf	443.84	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.86	J/mol×K	750.26	Joback Method
cpg	538.69	J/mol×K	790.87	Joback Method
cpg	551.29	J/mol×K	831.48	Joback Method
cpg	562.70	J/mol×K	872.09	Joback Method
cpg	572.96	J/mol×K	912.70	Joback Method
cpg	582.09	J/mol×K	953.30	Joback Method
cpg	590.13	J/mol×K	993.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375064&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