4-(Methylthio)benzoic acid, 2-fluoro-6-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C16H12F4O2S/c1-23-11-7-5-10(6-8-11)15(21)22-9-12-13(16(18,19)20)3-2-4-1

InchiKey: CHBKJHAAMVMKLN-UHFFFAOYSA-N

Formula: C16H12F4O2S

SMILES: CSc1ccc(C(=O)OCc2c(F)cccc2C(F)(F)F)cc1

Mol. weight [g/mol]: 344.32

Physical Properties

Property code	Value	Unit	Source
gf	-697.43	kJ/mol	Joback Method
hf	-931.04	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.923		Crippen Method
mcvol	219.650	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	772.70	K	Joback Method
tc	996.16	K	Joback Method
tf	471.82	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.36	J/mol×K	772.70	Joback Method
cpg	614.80	J/mol×K	809.94	Joback Method
cpg	626.16	J/mol×K	847.19	Joback Method
cpg	636.49	J/mol×K	884.43	Joback Method
cpg	645.82	J/mol×K	921.67	Joback Method
cpg	654.23	J/mol×K	958.92	Joback Method
cpg	661.74	J/mol×K	996.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375068&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