3-(Methylthio)benzoic pentafluoropropionic anhydride

Inchi: InChI=1S/C11H7F5O3S/c1-20-7-5-3-2-4-6(7)8(17)19-9(18)10(12,13)11(14,15)16/h2-5H,1

InchiKey: IGVIDERCMQOFIB-UHFFFAOYSA-N

Formula: C11H7F5O3S

SMILES: CSc1ccccc1C(=O)OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 314.23

Physical Properties

Property code	Value	Unit	Source
gf	-1153.57	kJ/mol	Joback Method
hf	-1358.87	kJ/mol	Joback Method
hfus	26.99	kJ/mol	Joback Method
hvap	59.06	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.289		Crippen Method
mcvol	176.300	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
tb	671.57	K	Joback Method
tc	880.94	K	Joback Method
tf	416.95	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.96	J/mol×K	671.57	Joback Method
cpg	469.43	J/mol×K	706.47	Joback Method
cpg	479.01	J/mol×K	741.36	Joback Method
cpg	487.73	J/mol×K	776.26	Joback Method
cpg	495.65	J/mol×K	811.15	Joback Method
cpg	502.81	J/mol×K	846.05	Joback Method
cpg	509.28	J/mol×K	880.94	Joback Method

Sources

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=U374987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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