4-(Trifluoroacetylthio)benzoic trifluoroacetic anhydride

Inchi: InChI=1S/C11H4F6O4S/c12-10(13,14)8(19)21-7(18)5-1-3-6(4-2-5)22-9(20)11(15,16)17/h

InchiKey: RTNFQGVFRFJNLE-UHFFFAOYSA-N

Formula: C11H4F6O4S

SMILES: O=C(OC(=O)C(F)(F)F)c1ccc(SC(=O)C(F)(F)F)cc1

Mol. weight [g/mol]: 346.20

Physical Properties

Property code	Value	Unit	Source
gf	-1477.30	kJ/mol	Joback Method
hf	-1667.56	kJ/mol	Joback Method
hfus	31.67	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.113		Crippen Method
mcvol	179.640	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1342.00		NIST Webbook
tb	724.71	K	Joback Method
tc	932.17	K	Joback Method
tf	467.47	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.14	J/mol×K	724.71	Joback Method
cpg	484.54	J/mol×K	759.29	Joback Method
cpg	492.12	J/mol×K	793.86	Joback Method
cpg	498.92	J/mol×K	828.44	Joback Method
cpg	505.00	J/mol×K	863.02	Joback Method
cpg	510.38	J/mol×K	897.59	Joback Method
cpg	515.13	J/mol×K	932.17	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=U375192&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