2-(Trifluoromethyl)thioxanthen-9-one

Other names: 2-(Trifluoromethyl)thioxanthen-9-one
2-(trifluoromethyl)-9H-thioxanthen-9-one
Inchi: InChI=1S/C14H7F3OS/c15-14(16,17)8-5-6-12-10(7-8)13(18)9-3-1-2-4-11(9)19-12/h1-7H
InchiKey: NEWRXGDGZGIHIS-UHFFFAOYSA-N
Formula: C14H7F3OS
SMILES: O=c1c2ccccc2sc2ccc(C(F)(F)F)cc12
Mol. weight [g/mol]: 280.27

Physical Properties

Property code	Value	Unit	Source
hf	-556.66	kJ/mol	Cheméo Relay (1.0)
hvap	97.88	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-5.26		Cheméo Relay (1.0)
logp	4.434		Crippen Method
mcvol	172.970	ml/mol	McGowan Method
tb	651.67	K	Cheméo Relay (1.0)
tf	426.38	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1693283&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point