2-Isopropylthioxanthone

Other names:	2-(1-methylethyl)-9H-thioxanthen-9-one
	2-isopropyl-9H-thioxanthen-9-one
	9H-Thioxanthen-9-one, 2-isopropyl
	Quantacure ITX
	Quantacure ITX (Isopropylthioxanthene-9-one)
Inchi:	InChI=1S/C16H14OS/c1-10(2)11-7-8-15-13(9-11)16(17)12-5-3-4-6-14(12)18-15/h3-10H,
InchiKey:	KTALPKYXQZGAEG-UHFFFAOYSA-N
Formula:	C16H14OS
SMILES:	CC(C)c1ccc2sc3ccccc3c(=O)c2c1
Mol. weight [g/mol]:	254.35

Physical Properties

Property code	Value	Unit	Source
hf	13.04	kJ/mol	Cheméo Relay (1.0)
hvap	109.00	kJ/mol	Cheméo Relay (1.0)
ie	7.91	eV	Cheméo Relay (1.0)
log10ws	-6.20		Cheméo Relay (1.0)
logp	4.538		Crippen Method
mcvol	195.840	ml/mol	McGowan Method
rinpol	2345.00		NIST Webbook
rinpol	2353.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	681.60	K	Cheméo Relay (1.0)
tf	399.57	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Determination and Correlation of Solubilities of 2-Isopropylthioxanthone (ITX) in Seven Different Solvents from (299.15 to 329.85) K:	https://www.doi.org/10.1021/je501011t
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5495841&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point