FURFURYL SULFIDE

Other names:	Difurfuryl sulfide
	Furan, 2,2'-[thiobis(methylene)]bis-
	2-([(2-Furylmethyl)sulfanyl]methyl)furan
	2-Difurfuryl sulfide
	bis(2-Furylmethyl) sulfide
	bis-Furfuryl sulfide
	di-2-Furfuryl sulfide
	2,2'-[thiobis(methylene)]bisfuran
Inchi:	InChI=1S/C10H10O2S/c1-3-9(11-5-1)7-13-8-10-4-2-6-12-10/h1-6H,7-8H2
InchiKey:	UYLKDZXJEKFFHJ-UHFFFAOYSA-N
Formula:	C10H10O2S
SMILES:	c1coc(CSCc2ccco2)c1
Mol. weight [g/mol]:	194.26

Physical Properties

Property code	Value	Unit	Source
hf	-52.42	kJ/mol	Cheméo Relay (1.0)
hvap	77.74	kJ/mol	Cheméo Relay (1.0)
ie	8.17	eV	Cheméo Relay (1.0)
logp	3.306		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
rinpol	1468.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1416.00		NIST Webbook
ripol	2223.00		NIST Webbook
ripol	2178.00		NIST Webbook
tb	549.58	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13678676&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature