2-FURANMETHANETHIOL, 5-METHYL-

Other names:	(5-Methyl-2-furyl)methanethiol
	2-Methyl-5-thiomethylfuran
	5-Methyl-2-furfurylmercaptan
	5-Methyl-2-furfurylthiol
	5-Methylfurfuryl mercaptan
Inchi:	InChI=1S/C6H8OS/c1-5-2-3-6(4-8)7-5/h2-3,8H,4H2,1H3
InchiKey:	MGLMZOFGBDYNMH-UHFFFAOYSA-N
Formula:	C6H8OS
SMILES:	Cc1ccc(CS)o1
Mol. weight [g/mol]:	128.20

Physical Properties

Property code	Value	Unit	Source
hvap	53.88	kJ/mol	Cheméo Relay (1.0)
ie	8.25	eV	Cheméo Relay (1.0)
logp	2.018		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	993.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1473.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1500.00		NIST Webbook
tb	447.98	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59303058&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
Cheméo Relay (1.0):	

Legend

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