2-ACETYL-5-METHYLFURAN

Other names:	Ethanone, 1-(5-methyl-2-furanyl)-
	Furan, 2-acetyl-5-methyl-
	5-Methyl-2-acetylfuran
	Ketone, methyl 5-methyl-2-furyl
	2-Methyl-5-acetylfuran
	5-Acetyl-2-methylfuran
	2-Acetyl, 5-mefuran
	1-(5-methyl-2-furyl)ethan-1-one
Inchi:	InChI=1S/C7H8O2/c1-5-3-4-7(9-5)6(2)8/h3-4H,1-2H3
InchiKey:	KEFJLCGVTHRGAH-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	CC(=O)c1ccc(C)o1
Mol. weight [g/mol]:	124.14

Physical Properties

Property code	Value	Unit	Source
hvap	54.81	kJ/mol	Cheméo Relay (1.0)
ie	8.78	eV	Cheméo Relay (1.0)
logp	1.791		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
rinpol	1000.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1038.80		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1038.80		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	1039.00		NIST Webbook

rinpol	1037.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	1004.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1571.00		NIST Webbook
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ripol	1609.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1571.00		NIST Webbook
tb	462.80	K	Cheméo Relay (1.0)
tf	302.39	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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1193799&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tf:	Normal melting (fusion) point